



## wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 12:44 PM JST

PDB ID : 6M16  
EMDB ID : EMD-30038  
Title : Cryo-EM structures of SARS-CoV spike glycoproteins  
Authors : Wang, X.; Yu, J.; Qiao, S.; Guo, R.  
Deposited on : 2020-02-24  
Resolution : 2.83 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

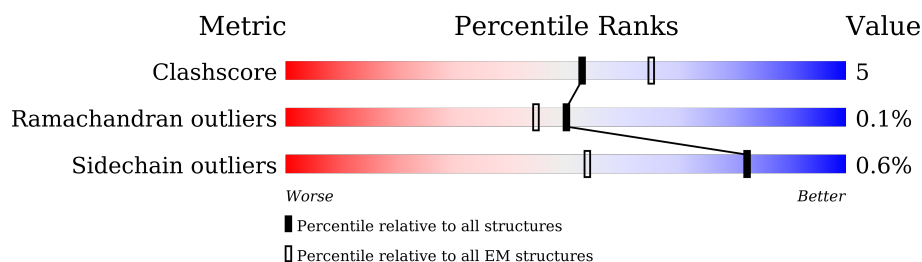
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1120	 75% 11% 14%
1	B	1120	 75% 11% 14%
1	C	1120	 75% 11% 14%
2	D	2	 50% 50%
2	E	2	 50% 50%
2	F	2	 50% 50%
2	H	2	 50% 50%
2	I	2	 50% 50%

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Mol	Chain	Length	Quality of chain
2	J	2	 50%50%
2	L	2	 50%50%
2	M	2	 50%50%
2	N	2	 50%50%
3	G	3	 67%33%
3	K	3	 67%33%
3	O	3	 67%33%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23433 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	B	965	Total	C	N	O	S	0	0
			7534	4787	1277	1424	46		
1	A	965	Total	C	N	O	S	0	0
			7534	4787	1277	1424	46		
1	C	965	Total	C	N	O	S	0	0
			7534	4787	1277	1424	46		

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1069	LEU	-	expression tag	UNP A0A2P1G1L3
B	1070	GLU	-	expression tag	UNP A0A2P1G1L3
B	1071	VAL	-	expression tag	UNP A0A2P1G1L3
B	1072	LEU	-	expression tag	UNP A0A2P1G1L3
B	1073	PHE	-	expression tag	UNP A0A2P1G1L3
B	1074	GLN	-	expression tag	UNP A0A2P1G1L3
B	1075	GLY	-	expression tag	UNP A0A2P1G1L3
B	1076	PRO	-	expression tag	UNP A0A2P1G1L3
B	1077	GLY	-	expression tag	UNP A0A2P1G1L3
B	1078	GLY	-	expression tag	UNP A0A2P1G1L3
B	1079	GLY	-	expression tag	UNP A0A2P1G1L3
B	1080	SER	-	expression tag	UNP A0A2P1G1L3
B	1081	GLY	-	expression tag	UNP A0A2P1G1L3
B	1082	GLY	-	expression tag	UNP A0A2P1G1L3
B	1083	GLY	-	expression tag	UNP A0A2P1G1L3
B	1084	SER	-	expression tag	UNP A0A2P1G1L3
B	1085	GLY	-	expression tag	UNP A0A2P1G1L3
B	1086	TYR	-	expression tag	UNP A0A2P1G1L3
B	1087	ILE	-	expression tag	UNP A0A2P1G1L3
B	1088	PRO	-	expression tag	UNP A0A2P1G1L3
B	1089	GLU	-	expression tag	UNP A0A2P1G1L3
B	1090	ALA	-	expression tag	UNP A0A2P1G1L3
B	1091	PRO	-	expression tag	UNP A0A2P1G1L3
B	1092	ARG	-	expression tag	UNP A0A2P1G1L3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1093	ASP	-	expression tag	UNP A0A2P1G1L3
B	1094	GLY	-	expression tag	UNP A0A2P1G1L3
B	1095	GLN	-	expression tag	UNP A0A2P1G1L3
B	1096	ALA	-	expression tag	UNP A0A2P1G1L3
B	1097	TYR	-	expression tag	UNP A0A2P1G1L3
B	1098	VAL	-	expression tag	UNP A0A2P1G1L3
B	1099	ARG	-	expression tag	UNP A0A2P1G1L3
B	1100	LYS	-	expression tag	UNP A0A2P1G1L3
B	1101	ASP	-	expression tag	UNP A0A2P1G1L3
B	1102	GLY	-	expression tag	UNP A0A2P1G1L3
B	1103	GLU	-	expression tag	UNP A0A2P1G1L3
B	1104	TRP	-	expression tag	UNP A0A2P1G1L3
B	1105	VAL	-	expression tag	UNP A0A2P1G1L3
B	1106	LEU	-	expression tag	UNP A0A2P1G1L3
B	1107	LEU	-	expression tag	UNP A0A2P1G1L3
B	1108	SER	-	expression tag	UNP A0A2P1G1L3
B	1109	THR	-	expression tag	UNP A0A2P1G1L3
B	1110	PHE	-	expression tag	UNP A0A2P1G1L3
B	1111	LEU	-	expression tag	UNP A0A2P1G1L3
B	1112	GLY	-	expression tag	UNP A0A2P1G1L3
B	1113	TRP	-	expression tag	UNP A0A2P1G1L3
B	1114	SER	-	expression tag	UNP A0A2P1G1L3
B	1115	HIS	-	expression tag	UNP A0A2P1G1L3
B	1116	PRO	-	expression tag	UNP A0A2P1G1L3
B	1117	GLN	-	expression tag	UNP A0A2P1G1L3
B	1118	PHE	-	expression tag	UNP A0A2P1G1L3
B	1119	GLU	-	expression tag	UNP A0A2P1G1L3
B	1120	LYS	-	expression tag	UNP A0A2P1G1L3
A	1069	LEU	-	expression tag	UNP A0A2P1G1L3
A	1070	GLU	-	expression tag	UNP A0A2P1G1L3
A	1071	VAL	-	expression tag	UNP A0A2P1G1L3
A	1072	LEU	-	expression tag	UNP A0A2P1G1L3
A	1073	PHE	-	expression tag	UNP A0A2P1G1L3
A	1074	GLN	-	expression tag	UNP A0A2P1G1L3
A	1075	GLY	-	expression tag	UNP A0A2P1G1L3
A	1076	PRO	-	expression tag	UNP A0A2P1G1L3
A	1077	GLY	-	expression tag	UNP A0A2P1G1L3
A	1078	GLY	-	expression tag	UNP A0A2P1G1L3
A	1079	GLY	-	expression tag	UNP A0A2P1G1L3
A	1080	SER	-	expression tag	UNP A0A2P1G1L3
A	1081	GLY	-	expression tag	UNP A0A2P1G1L3
A	1082	GLY	-	expression tag	UNP A0A2P1G1L3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1083	GLY	-	expression tag	UNP A0A2P1G1L3
A	1084	SER	-	expression tag	UNP A0A2P1G1L3
A	1085	GLY	-	expression tag	UNP A0A2P1G1L3
A	1086	TYR	-	expression tag	UNP A0A2P1G1L3
A	1087	ILE	-	expression tag	UNP A0A2P1G1L3
A	1088	PRO	-	expression tag	UNP A0A2P1G1L3
A	1089	GLU	-	expression tag	UNP A0A2P1G1L3
A	1090	ALA	-	expression tag	UNP A0A2P1G1L3
A	1091	PRO	-	expression tag	UNP A0A2P1G1L3
A	1092	ARG	-	expression tag	UNP A0A2P1G1L3
A	1093	ASP	-	expression tag	UNP A0A2P1G1L3
A	1094	GLY	-	expression tag	UNP A0A2P1G1L3
A	1095	GLN	-	expression tag	UNP A0A2P1G1L3
A	1096	ALA	-	expression tag	UNP A0A2P1G1L3
A	1097	TYR	-	expression tag	UNP A0A2P1G1L3
A	1098	VAL	-	expression tag	UNP A0A2P1G1L3
A	1099	ARG	-	expression tag	UNP A0A2P1G1L3
A	1100	LYS	-	expression tag	UNP A0A2P1G1L3
A	1101	ASP	-	expression tag	UNP A0A2P1G1L3
A	1102	GLY	-	expression tag	UNP A0A2P1G1L3
A	1103	GLU	-	expression tag	UNP A0A2P1G1L3
A	1104	TRP	-	expression tag	UNP A0A2P1G1L3
A	1105	VAL	-	expression tag	UNP A0A2P1G1L3
A	1106	LEU	-	expression tag	UNP A0A2P1G1L3
A	1107	LEU	-	expression tag	UNP A0A2P1G1L3
A	1108	SER	-	expression tag	UNP A0A2P1G1L3
A	1109	THR	-	expression tag	UNP A0A2P1G1L3
A	1110	PHE	-	expression tag	UNP A0A2P1G1L3
A	1111	LEU	-	expression tag	UNP A0A2P1G1L3
A	1112	GLY	-	expression tag	UNP A0A2P1G1L3
A	1113	TRP	-	expression tag	UNP A0A2P1G1L3
A	1114	SER	-	expression tag	UNP A0A2P1G1L3
A	1115	HIS	-	expression tag	UNP A0A2P1G1L3
A	1116	PRO	-	expression tag	UNP A0A2P1G1L3
A	1117	GLN	-	expression tag	UNP A0A2P1G1L3
A	1118	PHE	-	expression tag	UNP A0A2P1G1L3
A	1119	GLU	-	expression tag	UNP A0A2P1G1L3
A	1120	LYS	-	expression tag	UNP A0A2P1G1L3
C	1069	LEU	-	expression tag	UNP A0A2P1G1L3
C	1070	GLU	-	expression tag	UNP A0A2P1G1L3
C	1071	VAL	-	expression tag	UNP A0A2P1G1L3
C	1072	LEU	-	expression tag	UNP A0A2P1G1L3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1073	PHE	-	expression tag	UNP A0A2P1G1L3
C	1074	GLN	-	expression tag	UNP A0A2P1G1L3
C	1075	GLY	-	expression tag	UNP A0A2P1G1L3
C	1076	PRO	-	expression tag	UNP A0A2P1G1L3
C	1077	GLY	-	expression tag	UNP A0A2P1G1L3
C	1078	GLY	-	expression tag	UNP A0A2P1G1L3
C	1079	GLY	-	expression tag	UNP A0A2P1G1L3
C	1080	SER	-	expression tag	UNP A0A2P1G1L3
C	1081	GLY	-	expression tag	UNP A0A2P1G1L3
C	1082	GLY	-	expression tag	UNP A0A2P1G1L3
C	1083	GLY	-	expression tag	UNP A0A2P1G1L3
C	1084	SER	-	expression tag	UNP A0A2P1G1L3
C	1085	GLY	-	expression tag	UNP A0A2P1G1L3
C	1086	TYR	-	expression tag	UNP A0A2P1G1L3
C	1087	ILE	-	expression tag	UNP A0A2P1G1L3
C	1088	PRO	-	expression tag	UNP A0A2P1G1L3
C	1089	GLU	-	expression tag	UNP A0A2P1G1L3
C	1090	ALA	-	expression tag	UNP A0A2P1G1L3
C	1091	PRO	-	expression tag	UNP A0A2P1G1L3
C	1092	ARG	-	expression tag	UNP A0A2P1G1L3
C	1093	ASP	-	expression tag	UNP A0A2P1G1L3
C	1094	GLY	-	expression tag	UNP A0A2P1G1L3
C	1095	GLN	-	expression tag	UNP A0A2P1G1L3
C	1096	ALA	-	expression tag	UNP A0A2P1G1L3
C	1097	TYR	-	expression tag	UNP A0A2P1G1L3
C	1098	VAL	-	expression tag	UNP A0A2P1G1L3
C	1099	ARG	-	expression tag	UNP A0A2P1G1L3
C	1100	LYS	-	expression tag	UNP A0A2P1G1L3
C	1101	ASP	-	expression tag	UNP A0A2P1G1L3
C	1102	GLY	-	expression tag	UNP A0A2P1G1L3
C	1103	GLU	-	expression tag	UNP A0A2P1G1L3
C	1104	TRP	-	expression tag	UNP A0A2P1G1L3
C	1105	VAL	-	expression tag	UNP A0A2P1G1L3
C	1106	LEU	-	expression tag	UNP A0A2P1G1L3
C	1107	LEU	-	expression tag	UNP A0A2P1G1L3
C	1108	SER	-	expression tag	UNP A0A2P1G1L3
C	1109	THR	-	expression tag	UNP A0A2P1G1L3
C	1110	PHE	-	expression tag	UNP A0A2P1G1L3
C	1111	LEU	-	expression tag	UNP A0A2P1G1L3
C	1112	GLY	-	expression tag	UNP A0A2P1G1L3
C	1113	TRP	-	expression tag	UNP A0A2P1G1L3
C	1114	SER	-	expression tag	UNP A0A2P1G1L3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1115	HIS	-	expression tag	UNP A0A2P1G1L3
C	1116	PRO	-	expression tag	UNP A0A2P1G1L3
C	1117	GLN	-	expression tag	UNP A0A2P1G1L3
C	1118	PHE	-	expression tag	UNP A0A2P1G1L3
C	1119	GLU	-	expression tag	UNP A0A2P1G1L3
C	1120	LYS	-	expression tag	UNP A0A2P1G1L3

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	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	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		

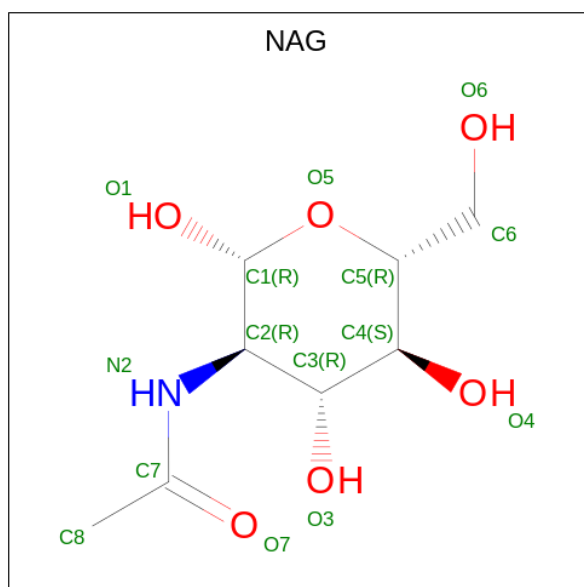
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

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





TRP
VAL
LEU
LEU
SER
THR
PHE
LEU
GLY
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

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

Chain D:  50% 50%

MAG1
MAG2

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

Chain E:  50% 50%

MAG1
MAG2

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

Chain F:  50% 50%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

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

Chain J:  50% 50%

MAG1
MAG2

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

Chain L:  50% 50%



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

Chain M:  50% 50%



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

Chain N:  50% 50%



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

Chain G:  67% 33%



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

Chain K:  67% 33%



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

Chain O:  67% 33%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152334	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.784	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.209	Depositor
Minimum map value	-0.150	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0201	Depositor
Map size ( $\text{\AA}$ )	271.616, 271.616, 271.616	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.061, 1.061, 1.061	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, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	0/7712	0.61	1/10499 (0.0%)
1	B	0.51	0/7712	0.61	1/10499 (0.0%)
1	C	0.51	0/7712	0.61	1/10499 (0.0%)
All	All	0.51	0/23136	0.61	3/31497 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
All	All	0	6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	LEU	CA-CB-CG	5.47	127.88	115.30
1	C	336	LEU	CA-CB-CG	5.46	127.86	115.30
1	B	336	LEU	CA-CB-CG	5.46	127.85	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	99	PRO	Peptide
1	B	118	ASN	Peptide
1	B	99	PRO	Peptide
1	C	99	PRO	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7534	0	7280	102	0
1	B	7534	0	7280	105	0
1	C	7534	0	7280	104	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	1	0
2	J	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	1	0
2	N	28	0	25	0	0
3	G	39	0	34	0	0
3	K	39	0	34	0	0
3	O	39	0	34	0	0
4	A	154	0	143	0	0
4	B	154	0	143	0	0
4	C	154	0	143	0	0
All	All	23433	0	22596	236	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 236 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:440:TYR:CE2	1:C:35:ARG:HD3	1.73	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:LEU:HD11	1:C:842:GLU:OE2	1.38	1.22
1:A:842:GLU:OE2	1:C:841:LEU:HD11	1.38	1.22
1:B:35:ARG:HD3	1:C:440:TYR:CE2	1.73	1.21
1:B:440:TYR:CE2	1:A:35:ARG:HD3	1.74	1.21

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	957/1120 (85%)	883 (92%)	73 (8%)	1 (0%)	48	69
1	B	957/1120 (85%)	884 (92%)	72 (8%)	1 (0%)	48	69
1	C	957/1120 (85%)	885 (92%)	71 (7%)	1 (0%)	48	69
All	All	2871/3360 (85%)	2652 (92%)	216 (8%)	3 (0%)	50	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	ILE
1	A	100	ILE
1	C	100	ILE

### 5.3.2 Protein sidechains [i](#)

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	832/967 (86%)	827 (99%)	5 (1%)	84	92
1	B	832/967 (86%)	827 (99%)	5 (1%)	84	92
1	C	832/967 (86%)	827 (99%)	5 (1%)	84	92
All	All	2496/2901 (86%)	2481 (99%)	15 (1%)	82	92

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	660	LEU
1	C	768	ASN
1	A	768	ASN
1	C	894	ASN
1	C	334	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	GLN
1	A	925	ASN
1	C	807	ASN
1	A	525	ASN
1	A	808	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

27 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	0.59	0	17,19,21	2.43	4 (23%)
2	NAG	D	2	2	14,14,15	0.32	0	17,19,21	0.47	0
2	NAG	E	1	2,1	14,14,15	0.38	0	17,19,21	0.76	1 (5%)
2	NAG	E	2	2	14,14,15	0.33	0	17,19,21	0.32	0
2	NAG	F	1	2,1	14,14,15	0.38	0	17,19,21	0.61	0
2	NAG	F	2	2	14,14,15	0.20	0	17,19,21	0.74	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.46	0	17,19,21	0.59	0
3	NAG	G	2	3	14,14,15	0.70	1 (7%)	17,19,21	0.65	0
3	BMA	G	3	3	11,11,12	0.84	0	15,15,17	0.81	0
2	NAG	H	1	2,1	14,14,15	0.59	0	17,19,21	2.43	4 (23%)
2	NAG	H	2	2	14,14,15	0.32	0	17,19,21	0.47	0
2	NAG	I	1	2,1	14,14,15	0.38	0	17,19,21	0.76	1 (5%)
2	NAG	I	2	2	14,14,15	0.33	0	17,19,21	0.32	0
2	NAG	J	1	2,1	14,14,15	0.38	0	17,19,21	0.61	0
2	NAG	J	2	2	14,14,15	0.21	0	17,19,21	0.74	1 (5%)
3	NAG	K	1	3,1	14,14,15	0.46	0	17,19,21	0.59	0
3	NAG	K	2	3	14,14,15	0.71	1 (7%)	17,19,21	0.65	0
3	BMA	K	3	3	11,11,12	0.84	0	15,15,17	0.81	0
2	NAG	L	1	2,1	14,14,15	0.59	0	17,19,21	2.43	3 (17%)
2	NAG	L	2	2	14,14,15	0.32	0	17,19,21	0.47	0
2	NAG	M	1	2,1	14,14,15	0.37	0	17,19,21	0.76	1 (5%)
2	NAG	M	2	2	14,14,15	0.33	0	17,19,21	0.32	0
2	NAG	N	1	2,1	14,14,15	0.38	0	17,19,21	0.60	0
2	NAG	N	2	2	14,14,15	0.19	0	17,19,21	0.73	1 (5%)
3	NAG	O	1	3,1	14,14,15	0.47	0	17,19,21	0.59	0
3	NAG	O	2	3	14,14,15	0.69	1 (7%)	17,19,21	0.65	0
3	BMA	O	3	3	11,11,12	0.83	0	15,15,17	0.81	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	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	BMA	O	3	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	2	NAG	O5-C1	-2.50	1.39	1.43
3	G	2	NAG	O5-C1	-2.47	1.39	1.43
3	O	2	NAG	O5-C1	-2.45	1.39	1.43

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1	NAG	C2-N2-C7	7.85	134.08	122.90
2	H	1	NAG	C2-N2-C7	7.84	134.07	122.90
2	D	1	NAG	C2-N2-C7	7.82	134.04	122.90
2	H	1	NAG	C1-C2-N2	4.55	118.26	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-C2-N2	4.55	118.25	110.49

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

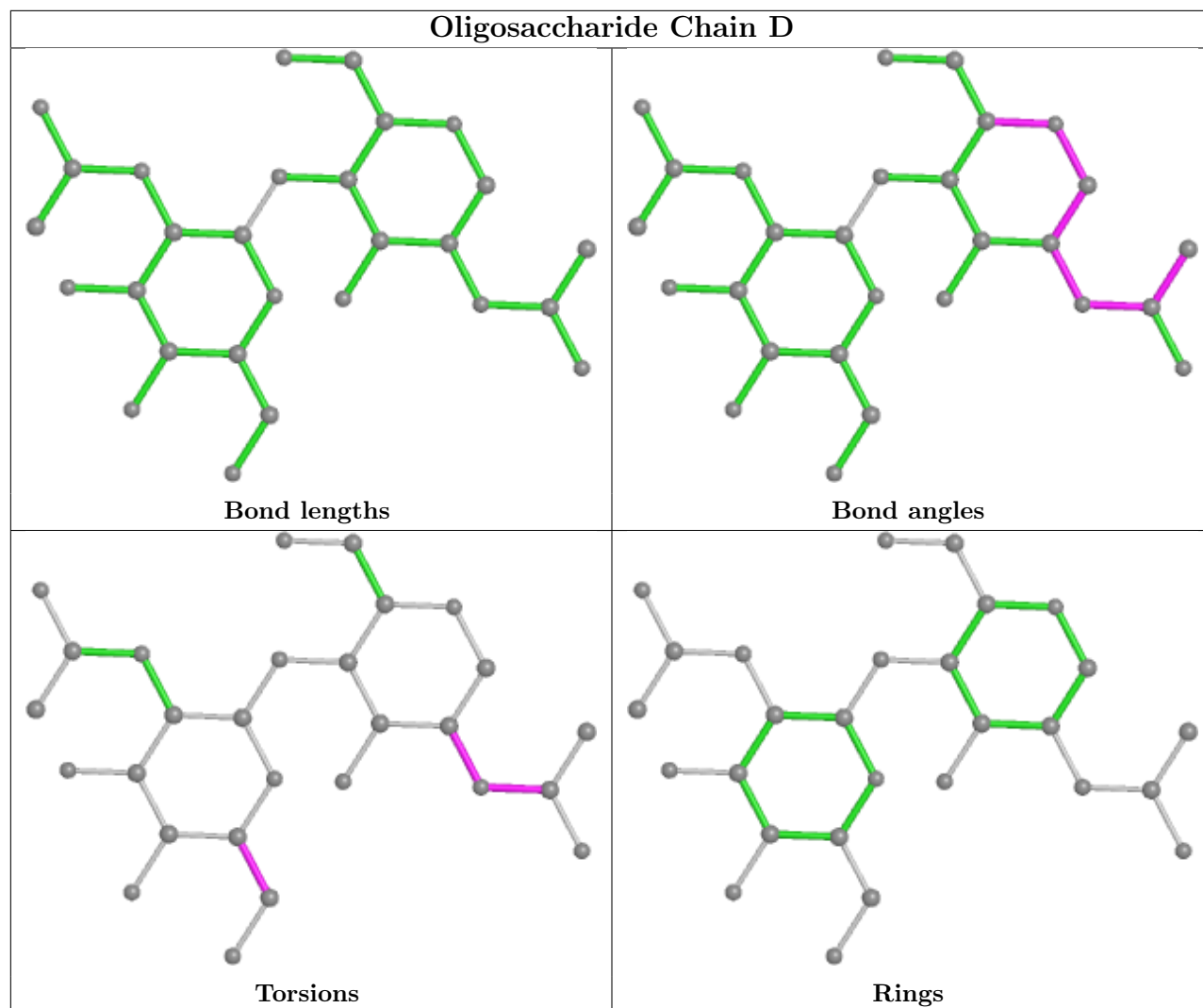
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	O5-C5-C6-O6
2	J	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6

There are no ring outliers.

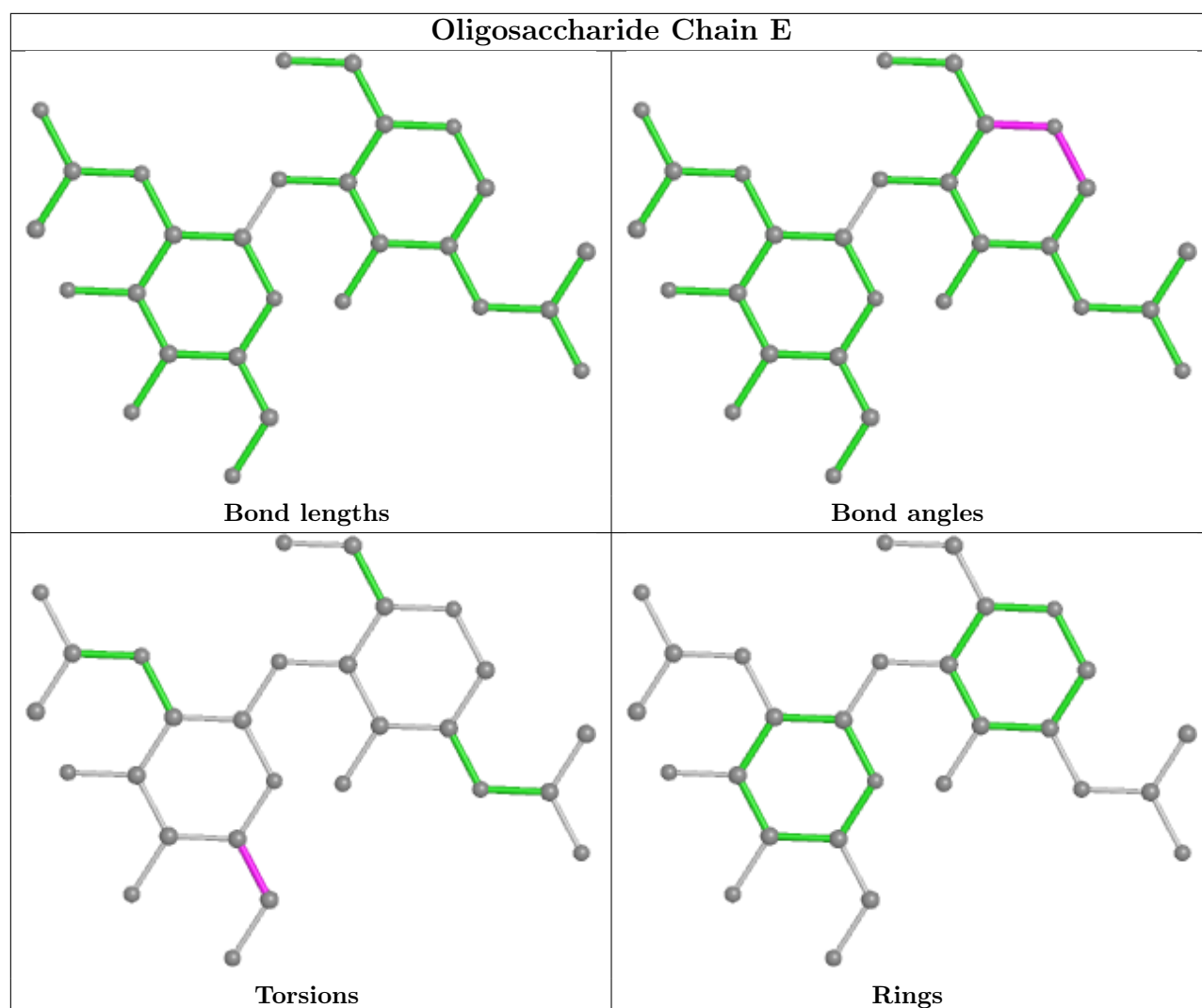
3 monomers are involved in 3 short contacts:

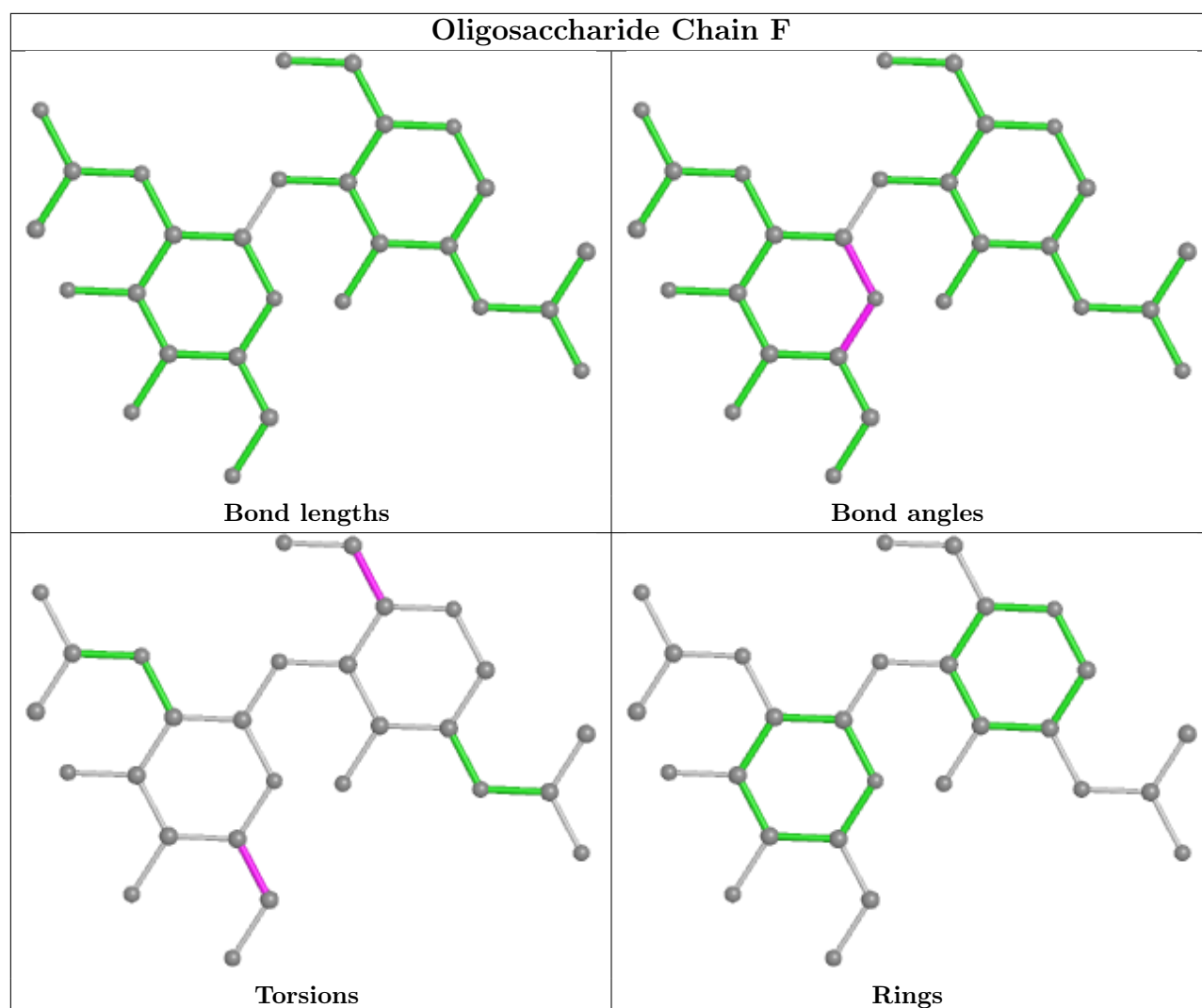
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	NAG	1	0
2	M	1	NAG	1	0
2	E	1	NAG	1	0

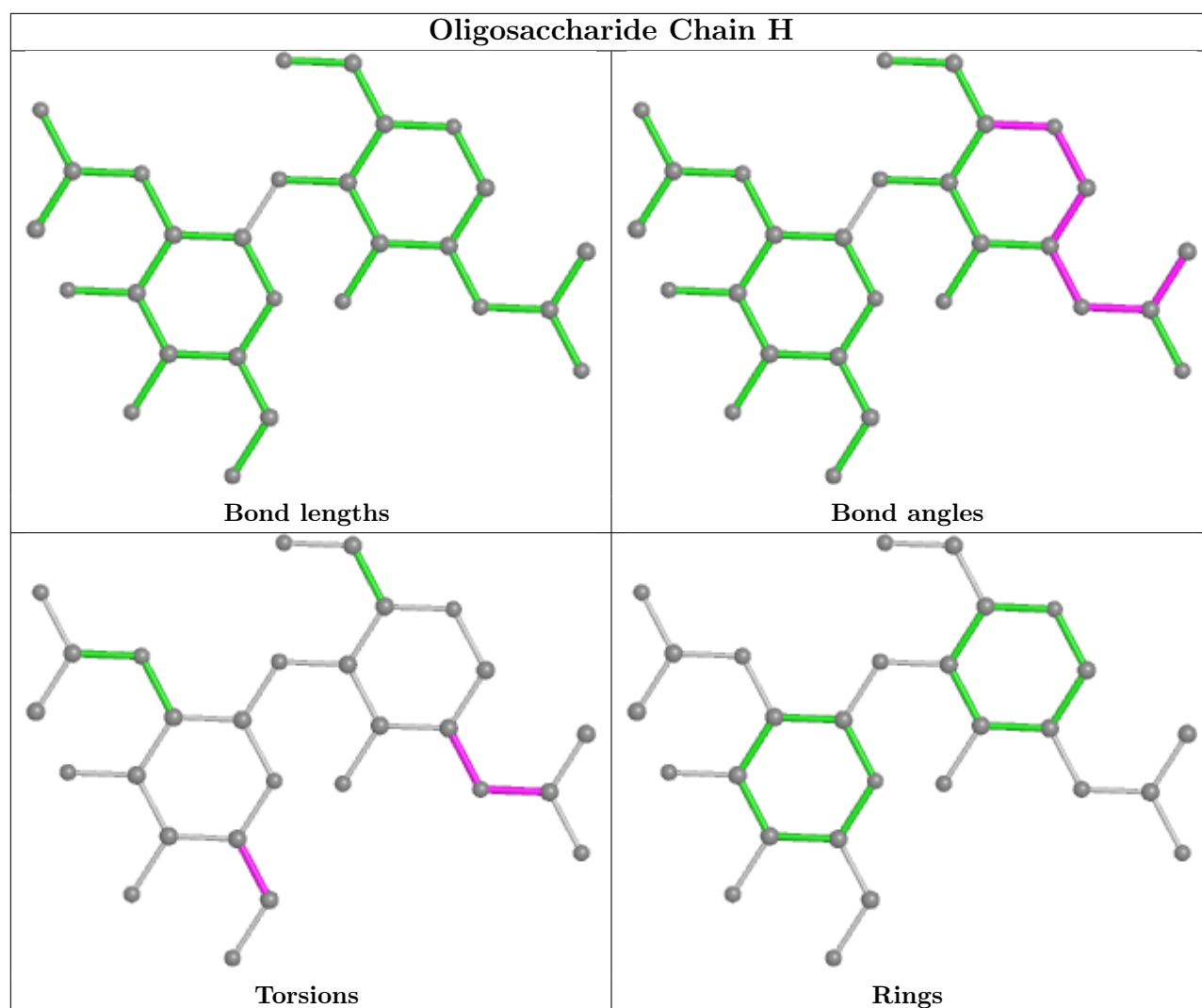
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

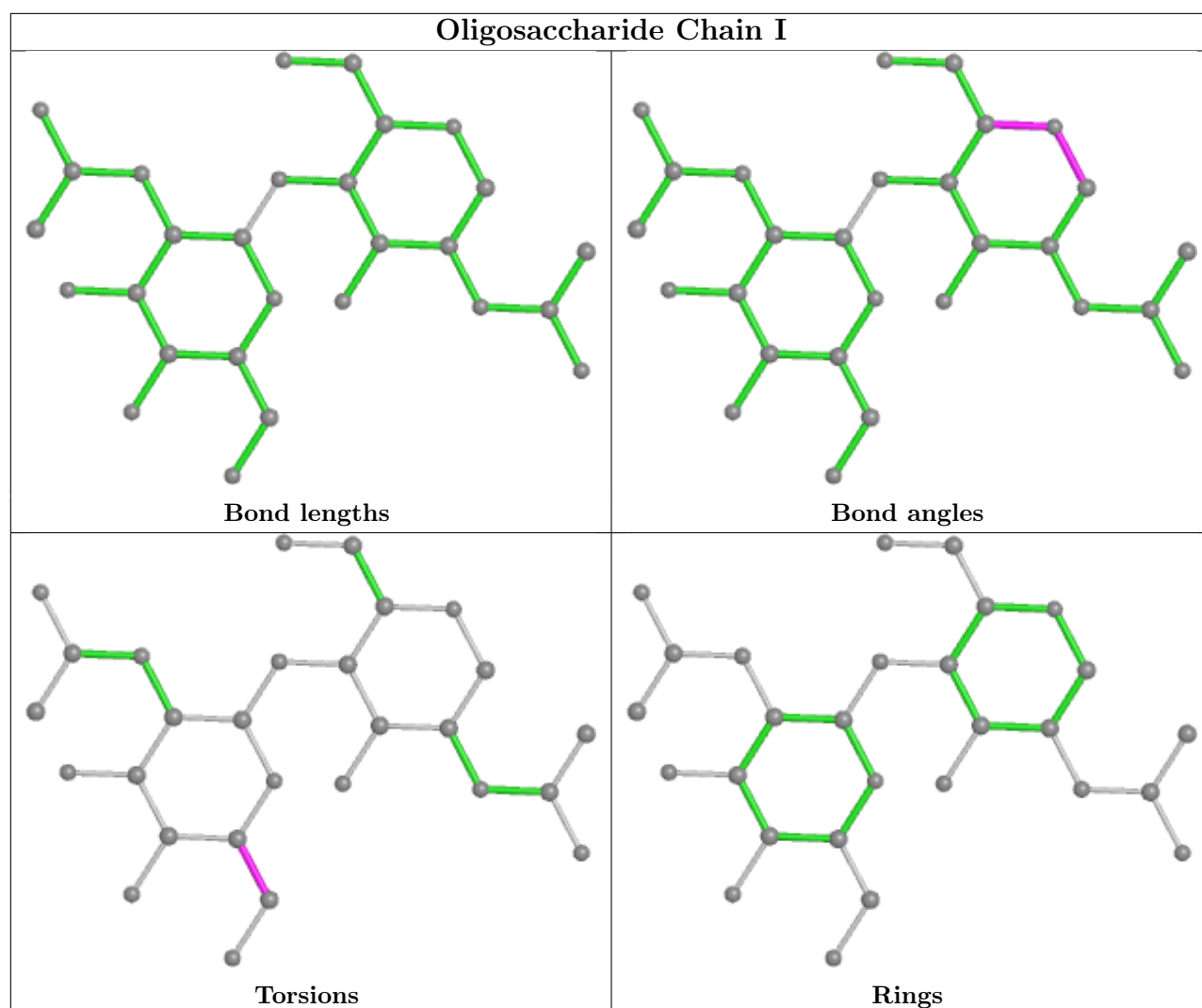


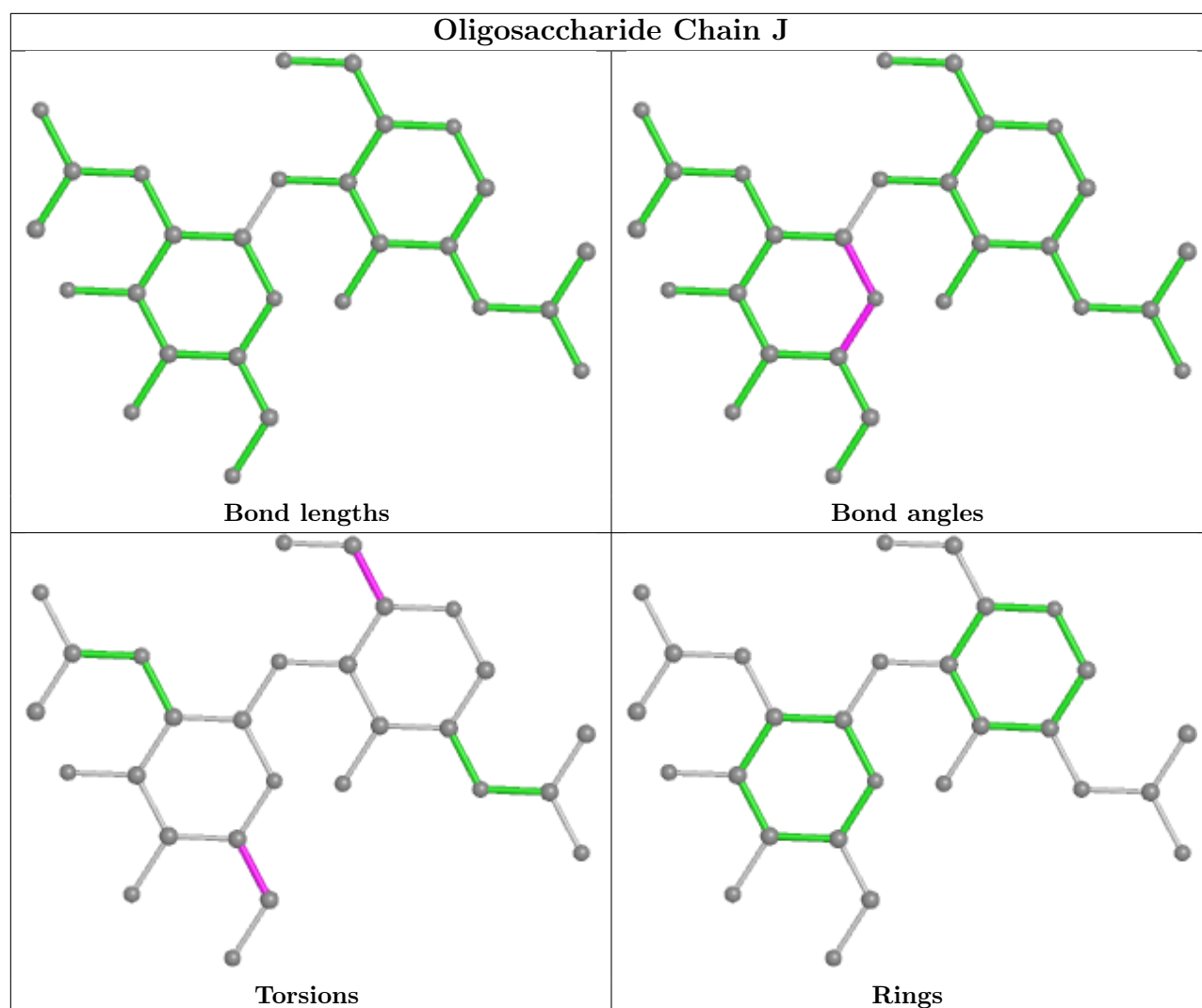


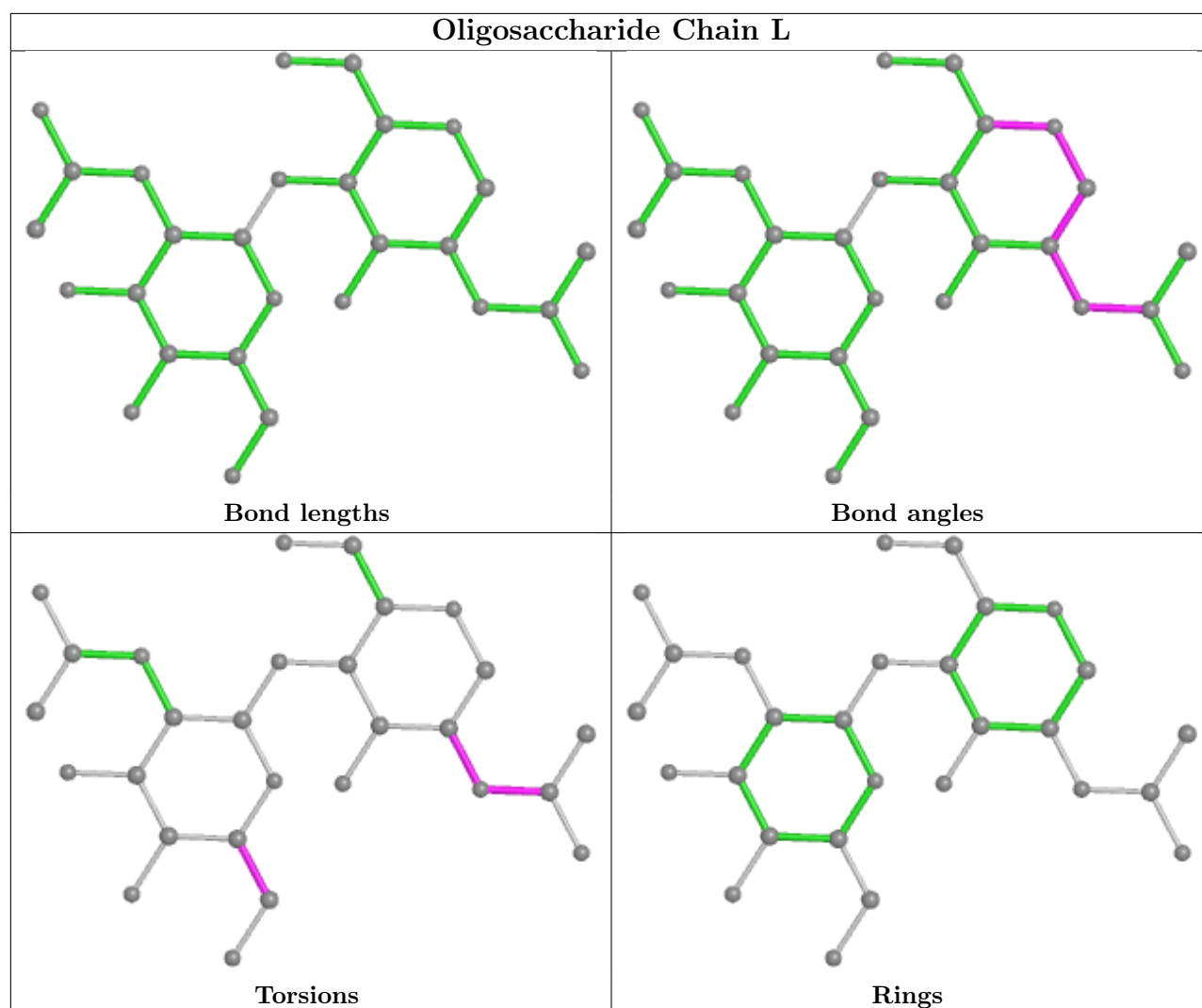


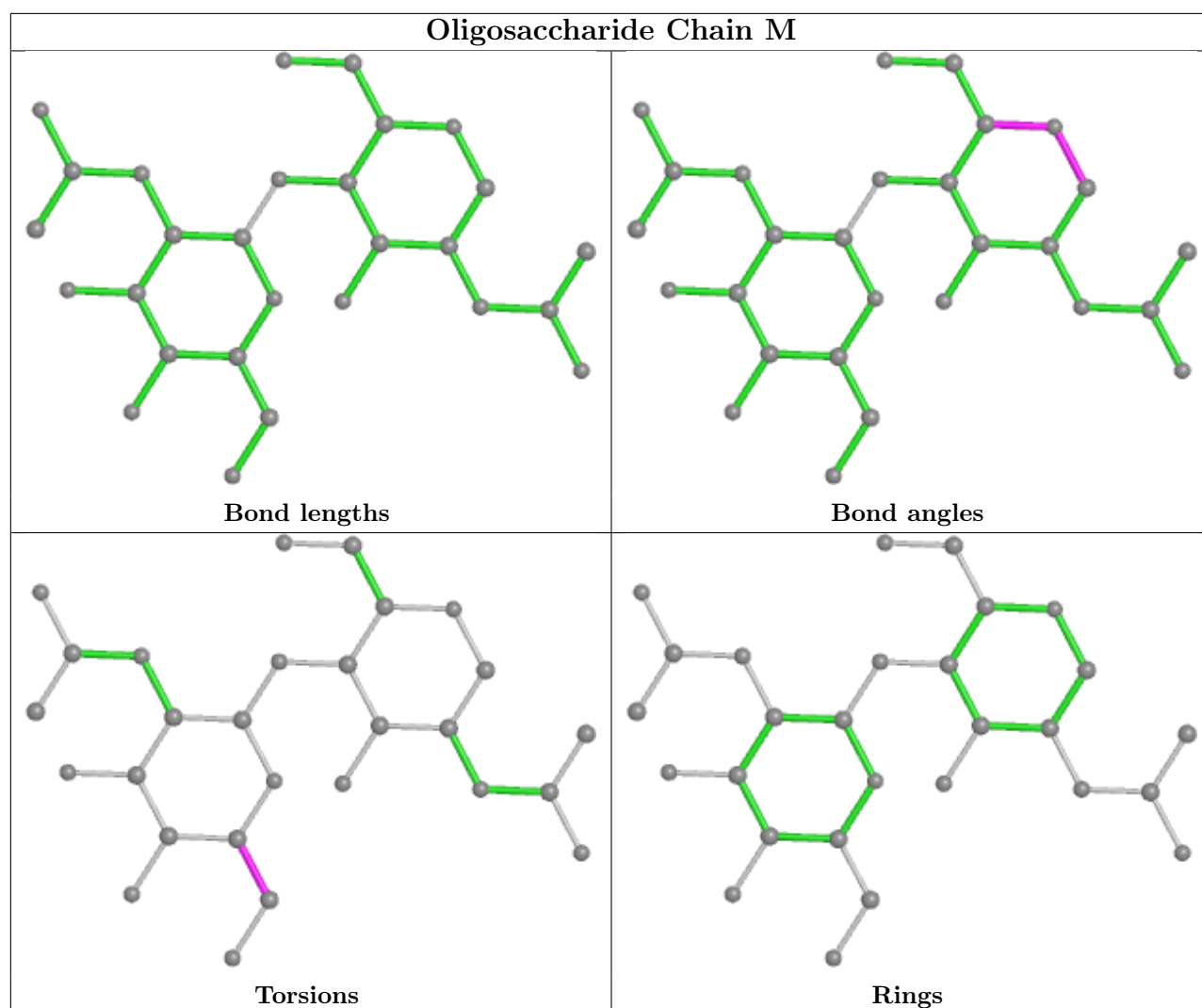


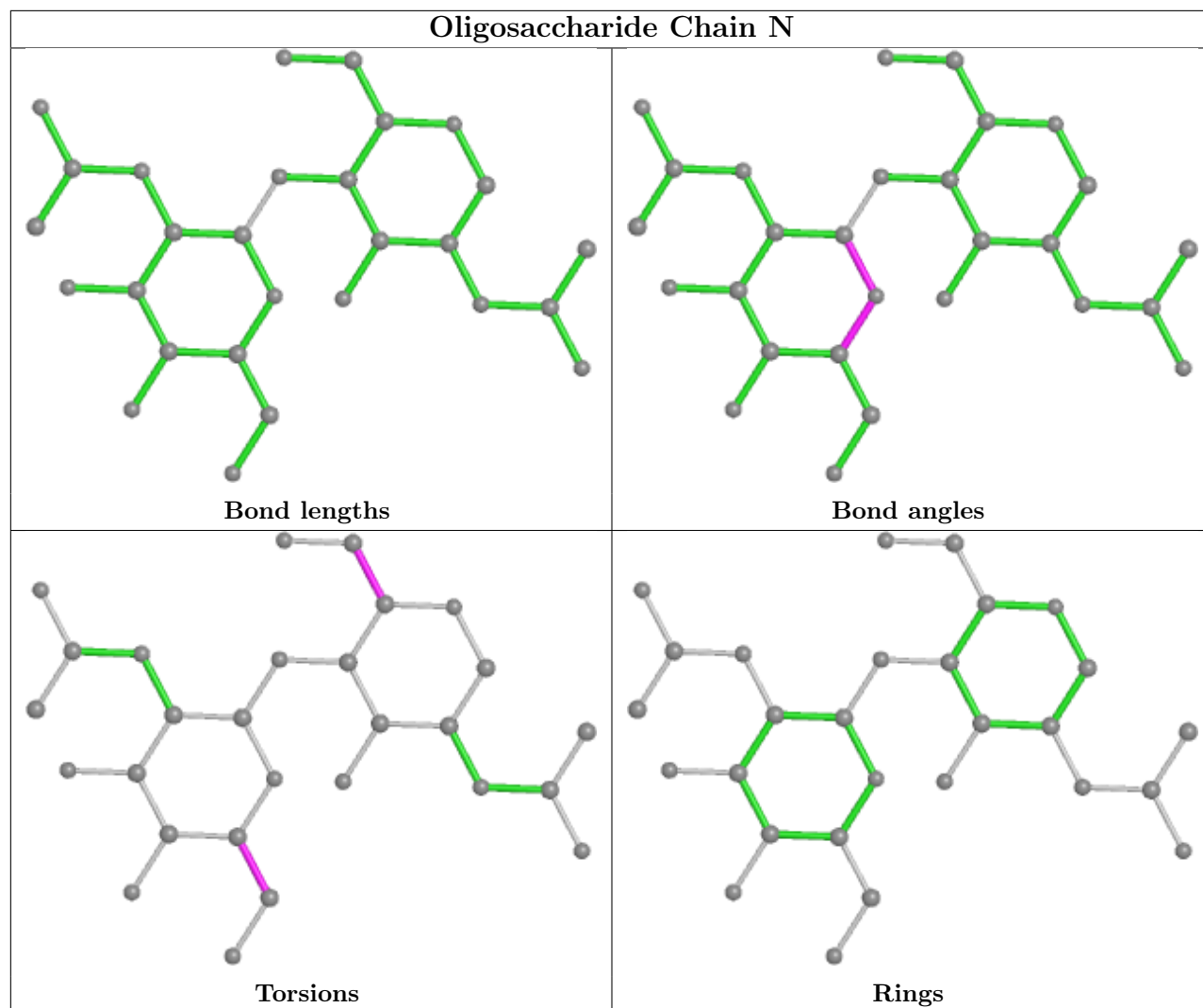




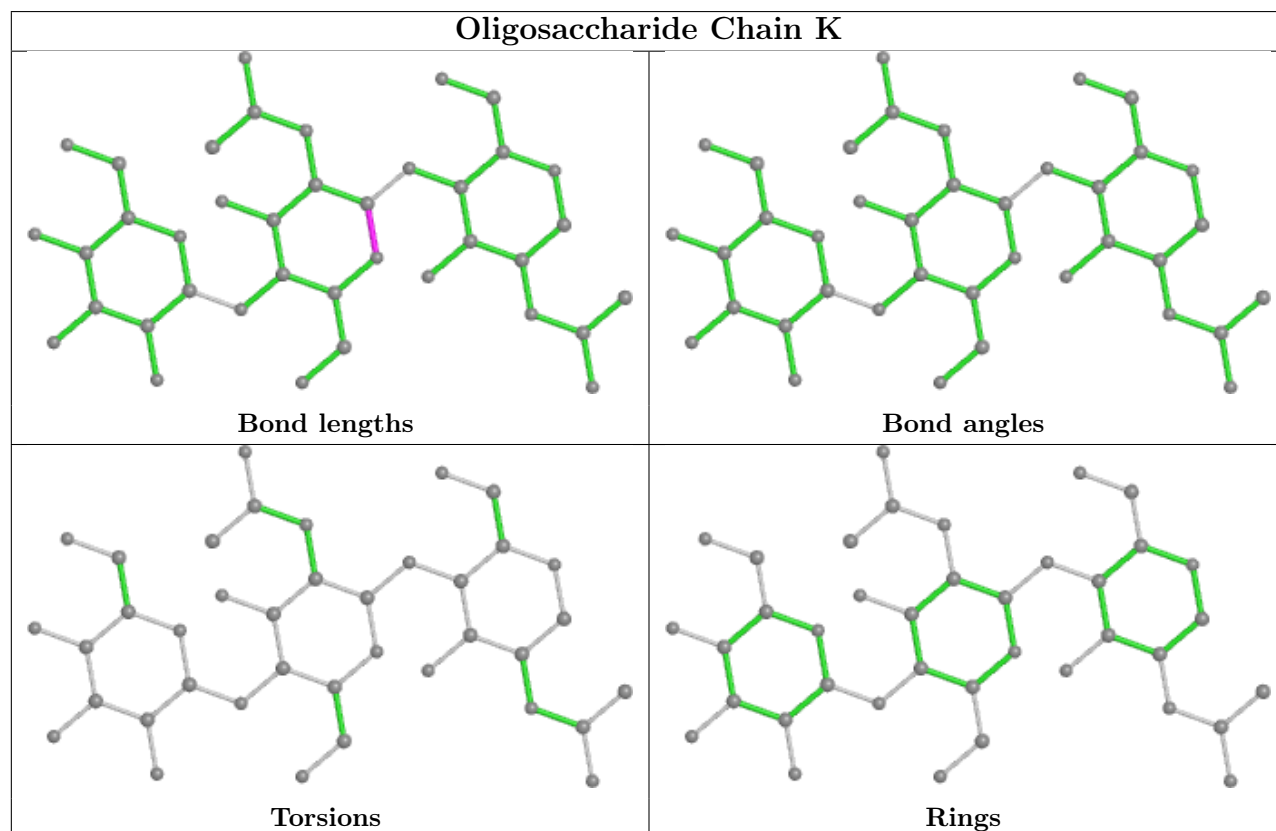
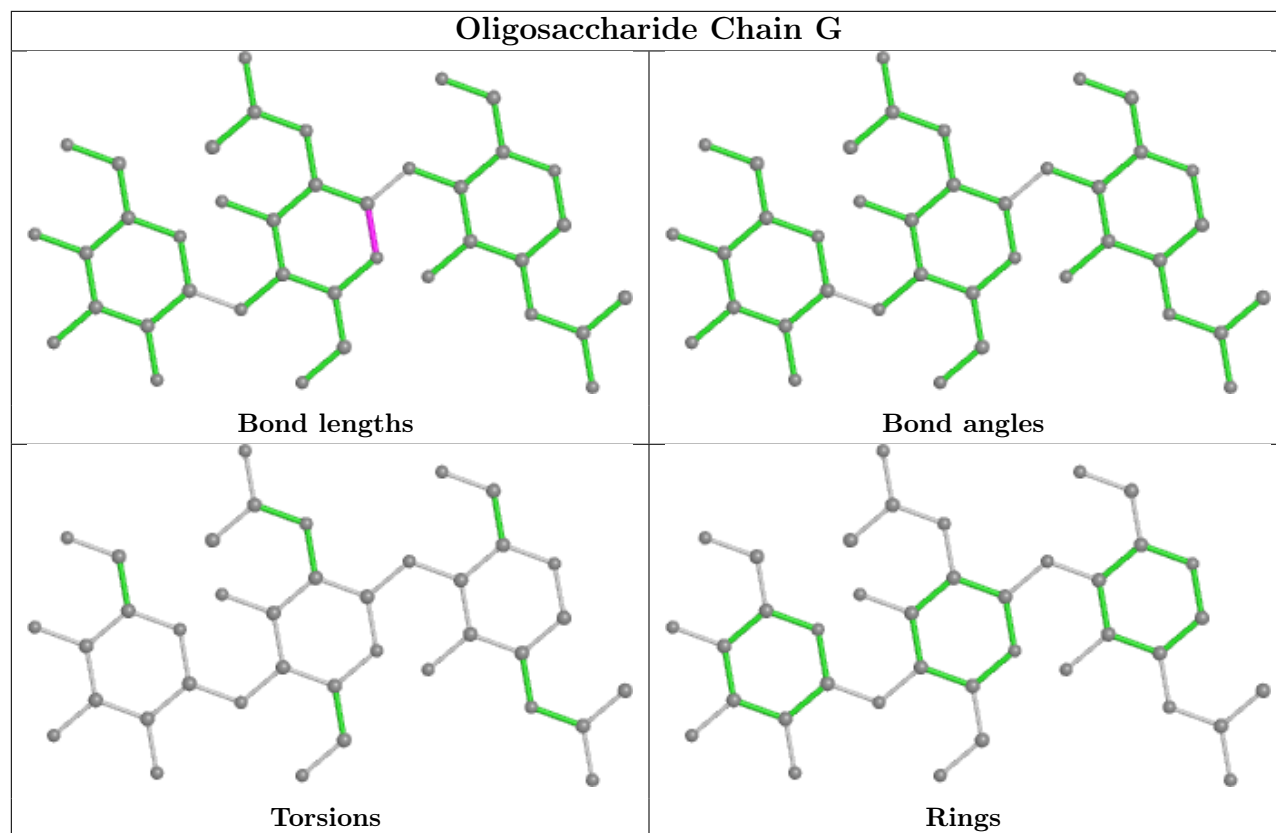


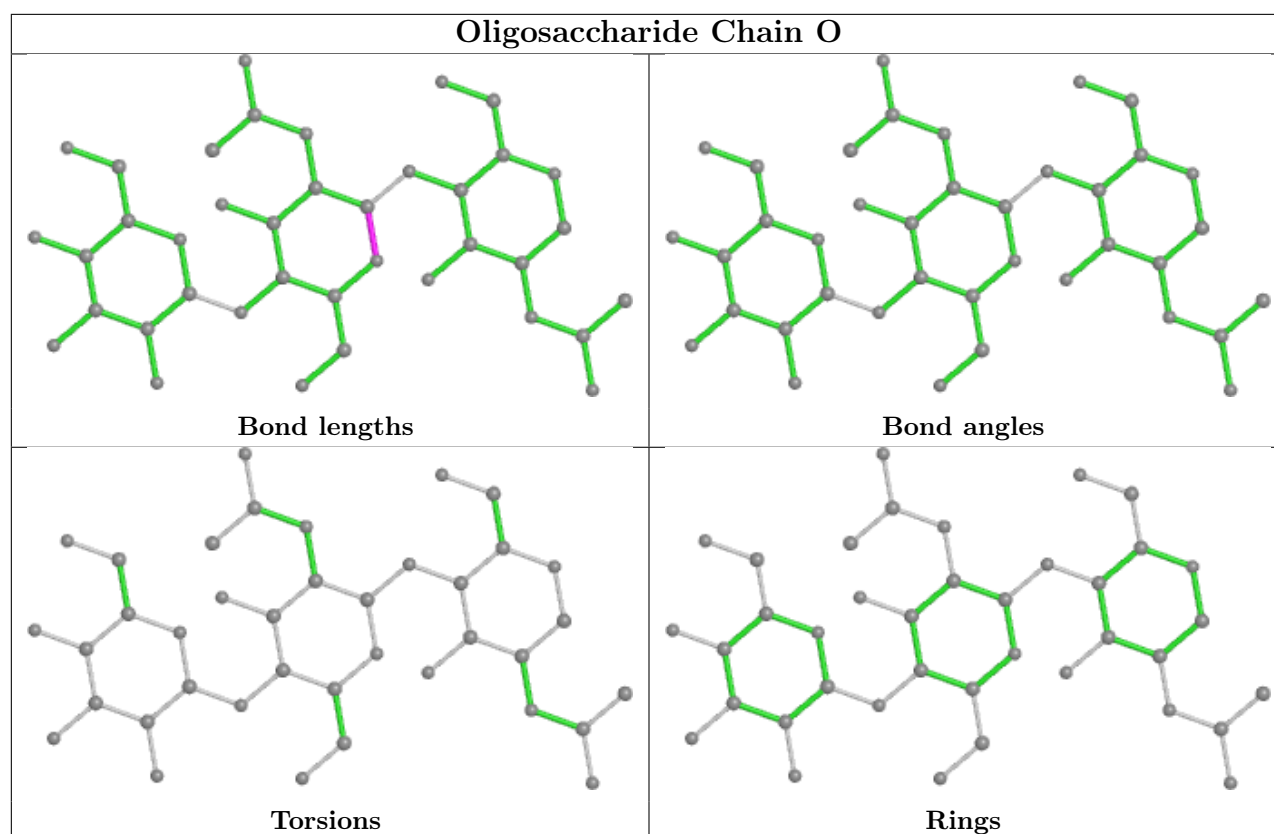












## 5.6 Ligand geometry [i](#)

33 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	C	1208	1	14,14,15	0.80	1 (7%)	17,19,21	1.14	1 (5%)
4	NAG	A	1216	-	14,14,15	0.37	0	17,19,21	0.38	0
4	NAG	C	1209	1	14,14,15	0.39	0	17,19,21	0.34	0
4	NAG	B	1208	1	14,14,15	0.80	1 (7%)	17,19,21	1.14	1 (5%)
4	NAG	B	1203	-	14,14,15	0.27	0	17,19,21	0.46	0
4	NAG	A	1205	1	14,14,15	0.43	0	17,19,21	0.53	0
4	NAG	B	1216	-	14,14,15	0.37	0	17,19,21	0.38	0
4	NAG	A	1209	1	14,14,15	0.39	0	17,19,21	0.35	0
4	NAG	A	1206	-	14,14,15	0.32	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	1206	-	14,14,15	0.33	0	17,19,21	0.41	0
4	NAG	C	1213	-	14,14,15	0.36	0	17,19,21	0.53	0
4	NAG	B	1209	1	14,14,15	0.39	0	17,19,21	0.35	0
4	NAG	B	1210	-	14,14,15	0.29	0	17,19,21	0.46	0
4	NAG	C	1216	-	14,14,15	0.37	0	17,19,21	0.38	0
4	NAG	A	1213	-	14,14,15	0.37	0	17,19,21	0.53	0
4	NAG	B	1213	-	14,14,15	0.36	0	17,19,21	0.53	0
4	NAG	A	1208	1	14,14,15	0.80	1 (7%)	17,19,21	1.14	1 (5%)
4	NAG	B	1205	1	14,14,15	0.43	0	17,19,21	0.53	0
4	NAG	A	1217	1	14,14,15	0.43	0	17,19,21	0.53	0
4	NAG	B	1207	-	14,14,15	0.34	0	17,19,21	0.53	0
4	NAG	A	1204	-	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	A	1210	-	14,14,15	0.30	0	17,19,21	0.46	0
4	NAG	B	1206	-	14,14,15	0.33	0	17,19,21	0.41	0
4	NAG	C	1207	-	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	C	1217	1	14,14,15	0.43	0	17,19,21	0.52	0
4	NAG	C	1204	-	14,14,15	0.28	0	17,19,21	0.60	0
4	NAG	C	1205	1	14,14,15	0.42	0	17,19,21	0.53	0
4	NAG	A	1207	-	14,14,15	0.34	0	17,19,21	0.54	0
4	NAG	B	1204	-	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	C	1203	-	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	A	1203	-	14,14,15	0.27	0	17,19,21	0.47	0
4	NAG	B	1217	1	14,14,15	0.43	0	17,19,21	0.52	0
4	NAG	C	1210	-	14,14,15	0.30	0	17,19,21	0.45	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	C	1208	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1216	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1209	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1208	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1203	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1205	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1216	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1209	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1206	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1206	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1213	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1209	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1210	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1216	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1213	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1213	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1208	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1205	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1217	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1207	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1204	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1210	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1206	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1207	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1217	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1204	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1205	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1207	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1204	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1203	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1203	-	-	1/6/23/26	0/1/1/1
4	NAG	B	1217	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1210	-	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1208	NAG	O5-C1	-2.40	1.39	1.43
4	A	1208	NAG	O5-C1	-2.39	1.39	1.43
4	B	1208	NAG	O5-C1	-2.39	1.39	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1208	NAG	C2-N2-C7	3.00	127.18	122.90
4	A	1208	NAG	C2-N2-C7	3.00	127.17	122.90
4	C	1208	NAG	C2-N2-C7	3.00	127.17	122.90

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1204	NAG	O5-C5-C6-O6
4	A	1204	NAG	O5-C5-C6-O6
4	C	1204	NAG	O5-C5-C6-O6
4	B	1206	NAG	O5-C5-C6-O6
4	A	1206	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

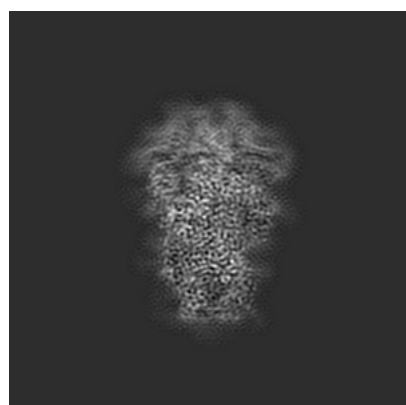
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30038. These allow visual inspection of the internal detail of the map and identification of artifacts.

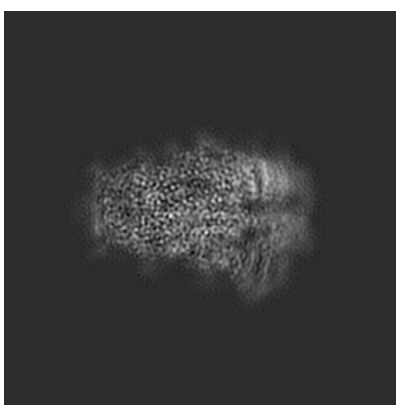
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

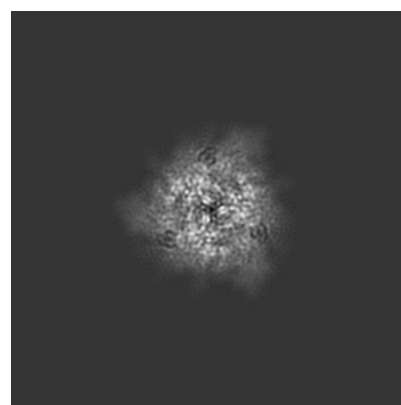
#### 6.1.1 Primary map



X



Y

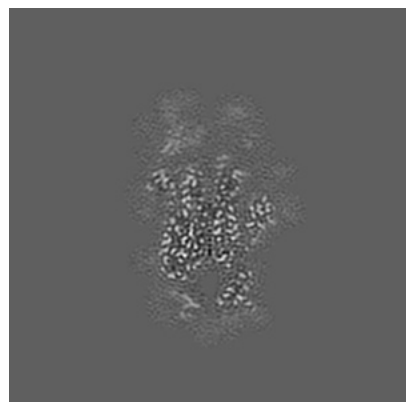


Z

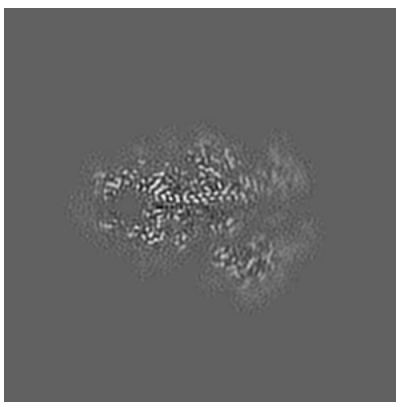
The images above show the map projected in three orthogonal directions.

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

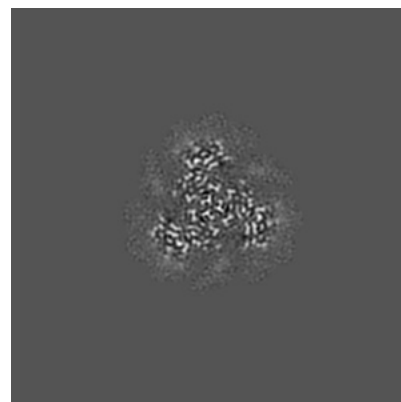
#### 6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

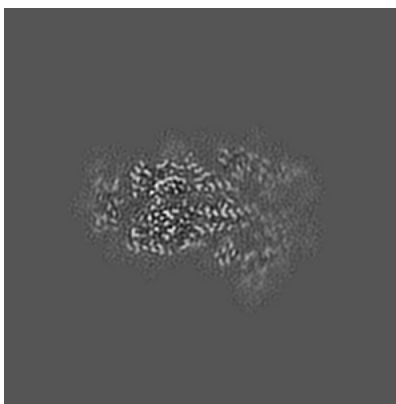
The images above show central slices of the map in three orthogonal directions.

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

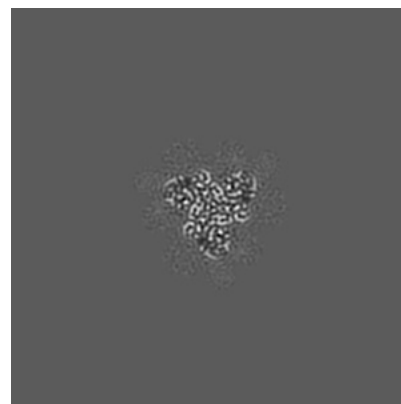
### 6.3.1 Primary map



X Index: 125



Y Index: 136

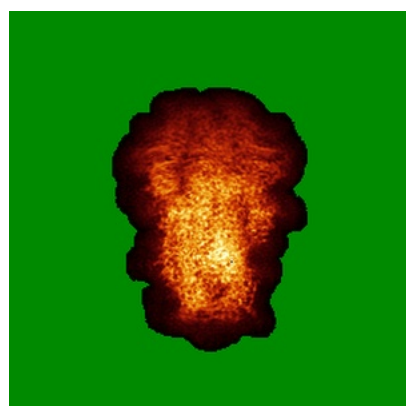


Z Index: 98

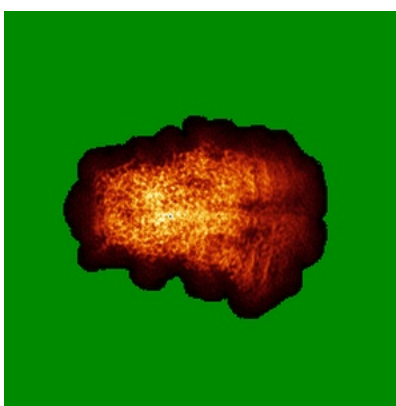
The images above show the largest variance slices of the map in three orthogonal directions.

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

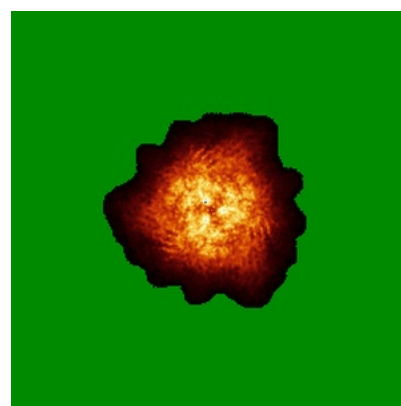
### 6.4.1 Primary map



X



Y

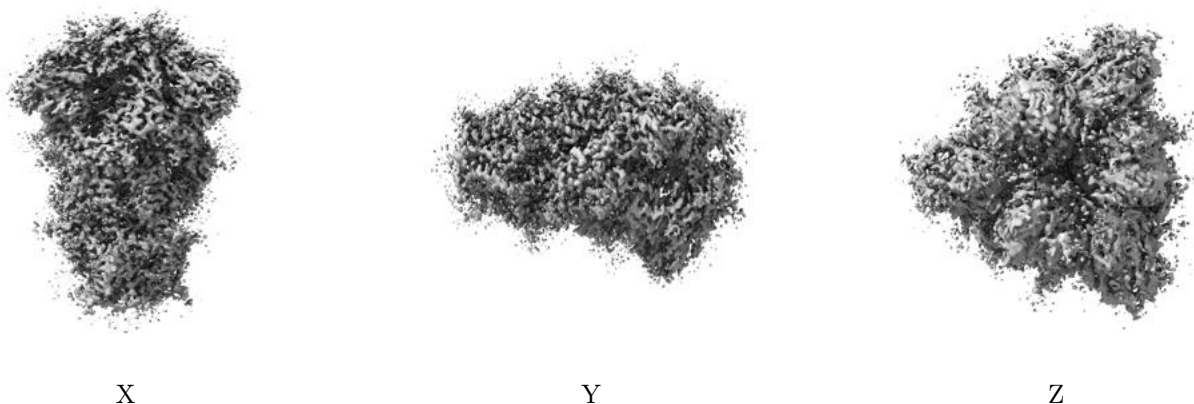


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0201. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation [i](#)

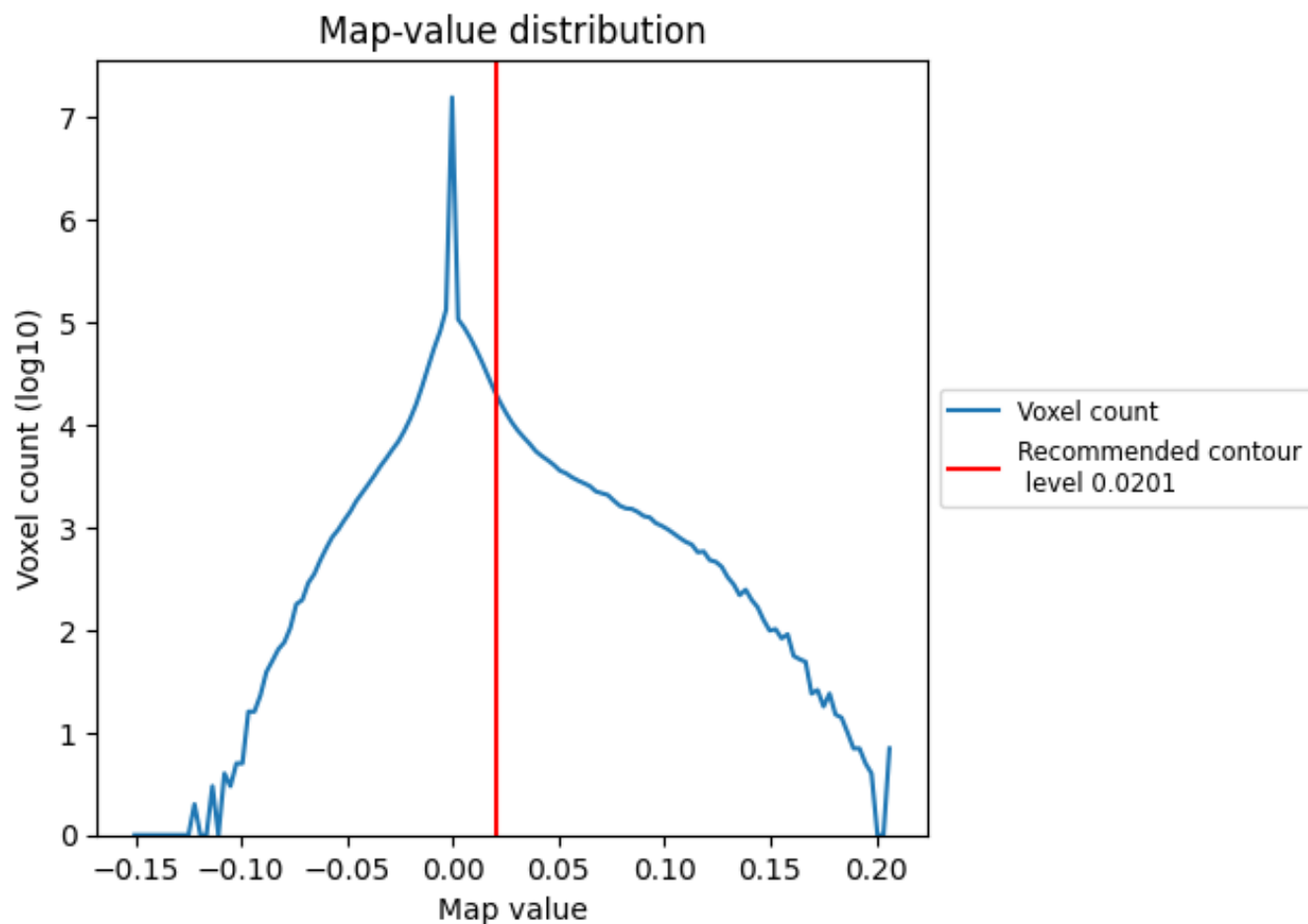
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

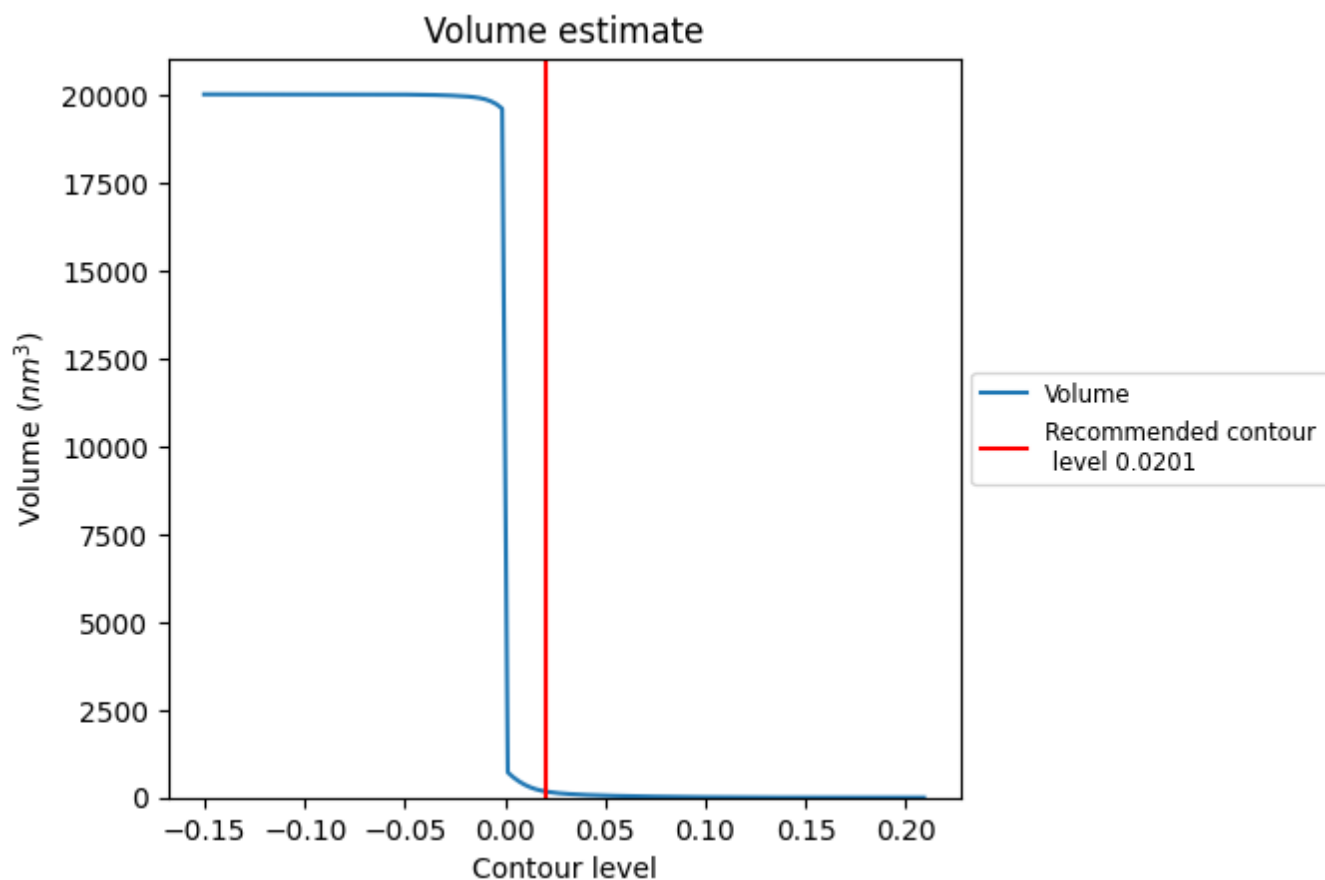
This section contains the results of statistical analysis of the map.

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



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

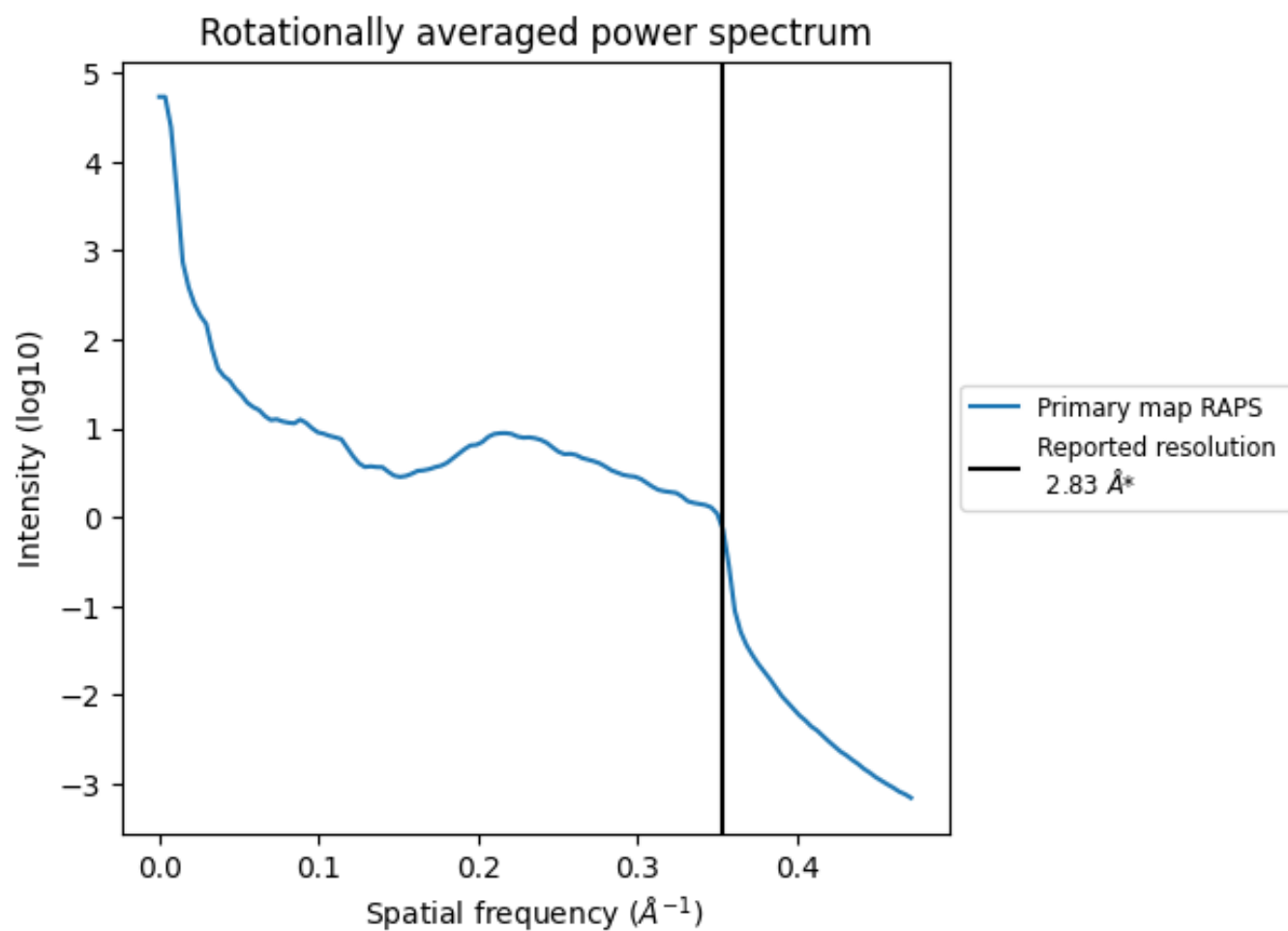
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 175 nm<sup>3</sup>; this corresponds to an approximate mass of 158 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 0.353 Å<sup>-1</sup>

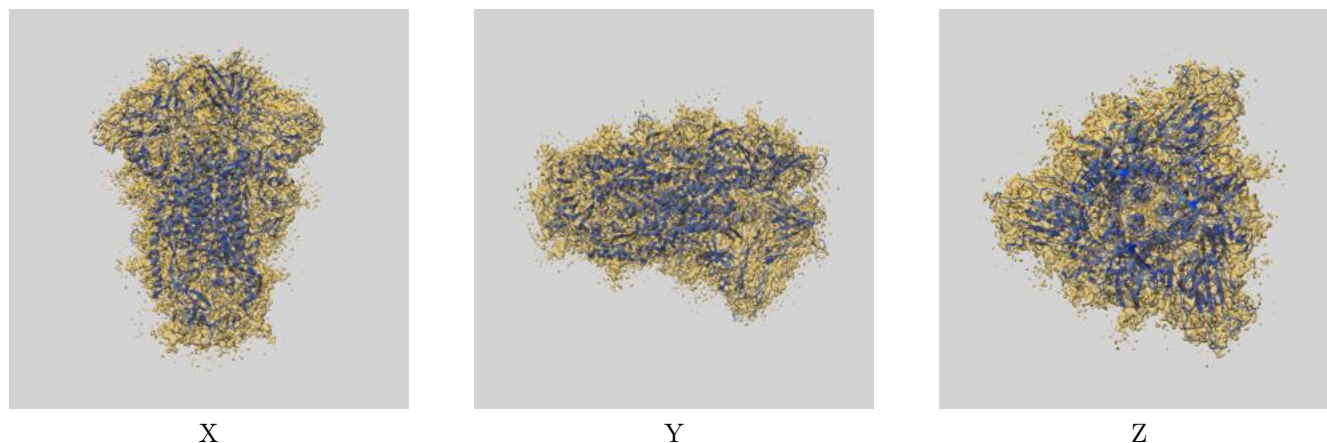
## 8 Fourier-Shell correlation

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

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

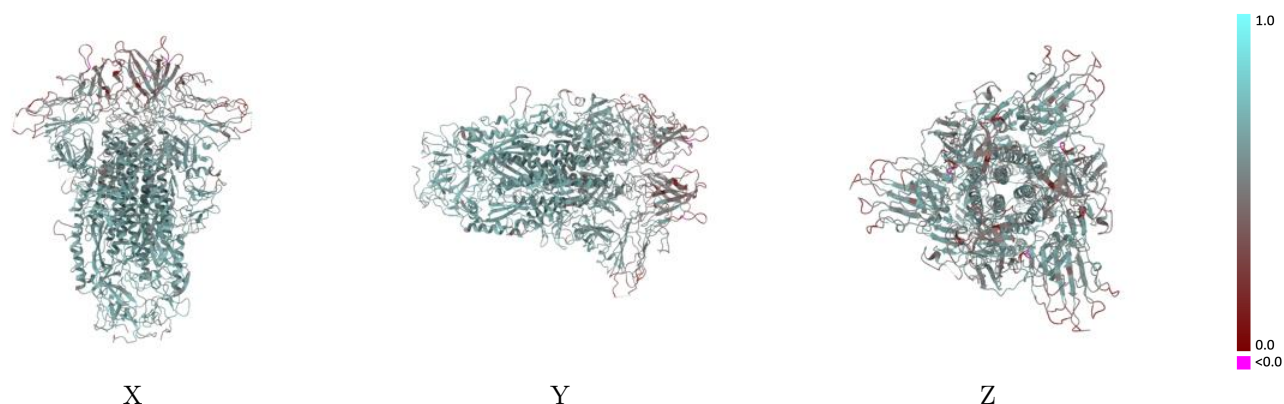
This section contains information regarding the fit between EMDB map EMD-30038 and PDB model 6M16. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

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



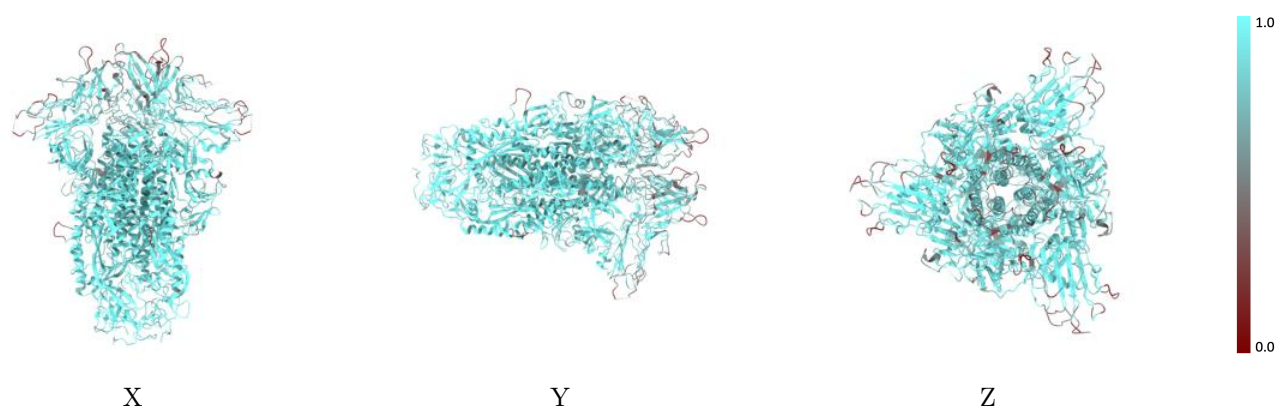
The images above show the 3D surface view of the map at the recommended contour level 0.0201 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



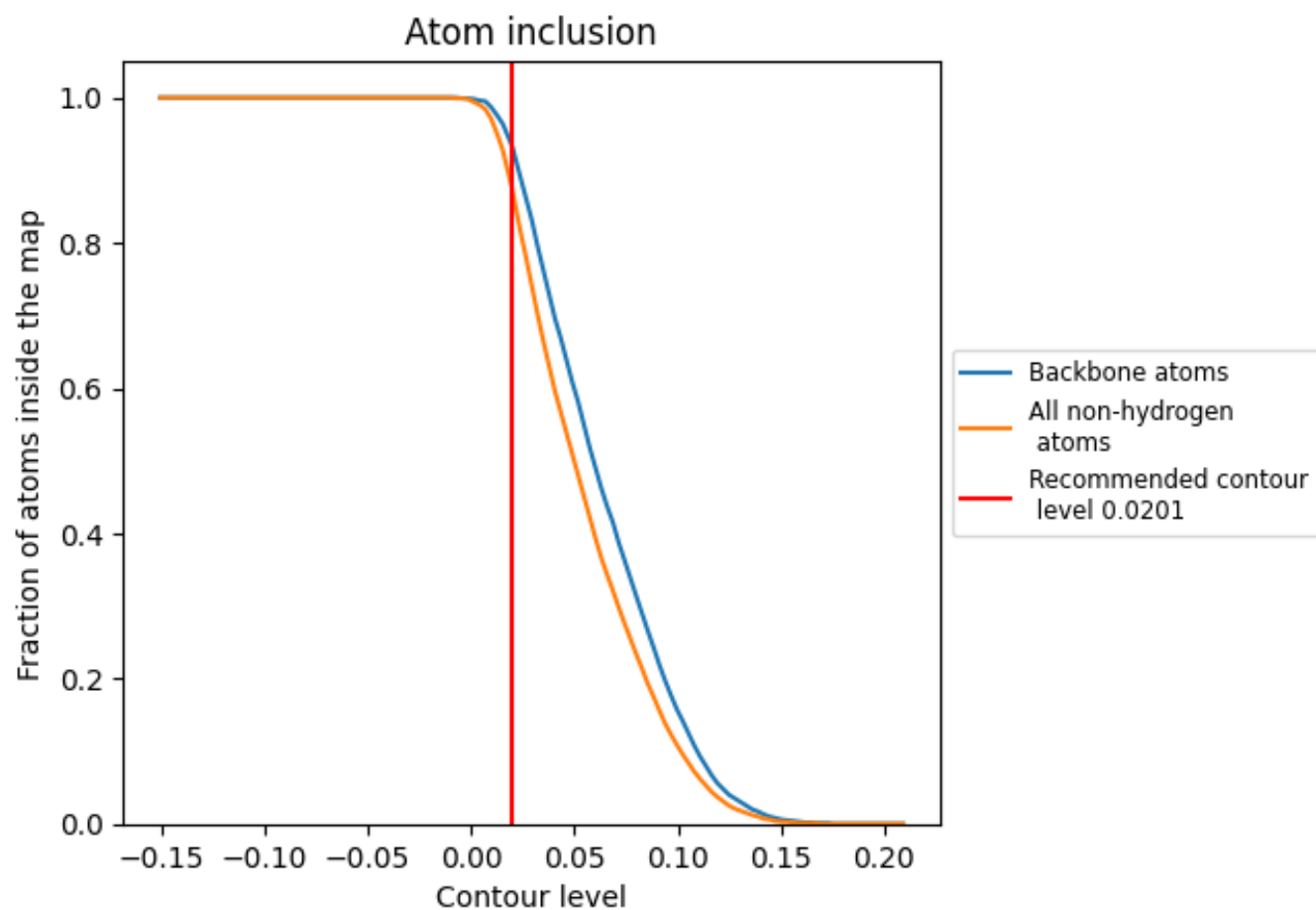
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0201).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% 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 (0.0201) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8730	<div><div></div></div> 0.5590
A	<div><div></div></div> 0.8710	<div><div></div></div> 0.5580
B	<div><div></div></div> 0.8750	<div><div></div></div> 0.5610
C	<div><div></div></div> 0.8720	<div><div></div></div> 0.5580
D	<div><div></div></div> 0.8930	<div><div></div></div> 0.5280
E	<div><div></div></div> 0.8930	<div><div></div></div> 0.5450
F	<div><div></div></div> 0.9640	<div><div></div></div> 0.5350
G	<div><div></div></div> 0.8970	<div><div></div></div> 0.5630
H	<div><div></div></div> 0.8930	<div><div></div></div> 0.5270
I	<div><div></div></div> 0.8570	<div><div></div></div> 0.5480
J	<div><div></div></div> 0.9640	<div><div></div></div> 0.5250
K	<div><div></div></div> 0.8970	<div><div></div></div> 0.5520
L	<div><div></div></div> 0.8930	<div><div></div></div> 0.5150
M	<div><div></div></div> 0.8570	<div><div></div></div> 0.5380
N	<div><div></div></div> 0.9640	<div><div></div></div> 0.5150
O	<div><div></div></div> 0.8970	<div><div></div></div> 0.5720

1.0

0.0

<0.0