



## Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 03:55 pm GMT

PDB ID : 6ZP0  
EMDB ID : EMD-11332  
Title : Structure of SARS-CoV-2 Spike Protein Trimer (single Arg S1/S2 cleavage site) in Closed State  
Authors : Xiong, X.; Qu, K.; Scheres, S.H.W.; Briggs, J.A.G.  
Deposited on : 2020-07-08  
Resolution : 3.00 Å (reported)  
Based on initial model : 6VXX

This is a Full wwPDB EM Validation 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.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

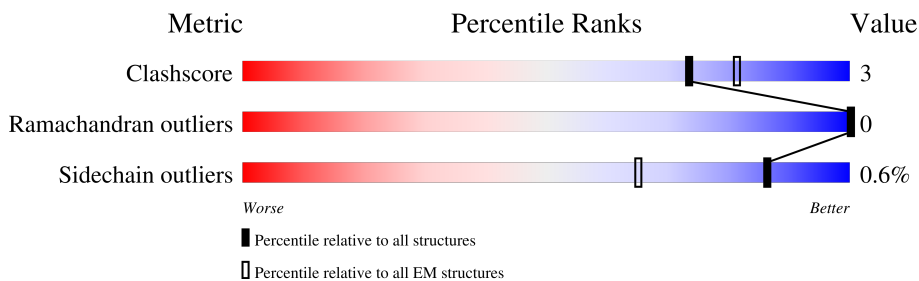
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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  $\geq 3$ , 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	1247	
1	B	1247	
1	C	1247	
2	D	2	
2	E	2	
2	F	2	
2	G	2	
2	H	2	

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Mol	Chain	Length	Quality of chain
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%
2	N	2	 100%
2	O	2	 100%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 24957 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
			Total	C	N	O	S		
1	A	1030	8039	5129	1337	1536	37	0	0
1	B	1030	8039	5129	1337	1536	37	0	0
1	C	1030	8039	5129	1337	1536	37	0	0

There are 171 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLU	-	expression tag	UNP P0DTC2
A	11	THR	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	THR	-	expression tag	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	1212	GLY	-	expression tag	UNP P0DTC2
A	1213	SER	-	expression tag	UNP P0DTC2
A	1214	GLY	-	expression tag	UNP P0DTC2
A	1215	ARG	-	expression tag	UNP P0DTC2
A	1216	GLU	-	expression tag	UNP P0DTC2
A	1217	ASN	-	expression tag	UNP P0DTC2
A	1218	LEU	-	expression tag	UNP P0DTC2
A	1219	TYR	-	expression tag	UNP P0DTC2
A	1220	PHE	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLY	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	TYR	-	expression tag	UNP P0DTC2
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	ASP	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
A	1241	ARG	-	expression tag	UNP P0DTC2
A	1242	LYS	-	expression tag	UNP P0DTC2
A	1243	ASP	-	expression tag	UNP P0DTC2
A	1244	GLY	-	expression tag	UNP P0DTC2
A	1245	GLU	-	expression tag	UNP P0DTC2
A	1246	TRP	-	expression tag	UNP P0DTC2
A	1247	VAL	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	LEU	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	THR	-	expression tag	UNP P0DTC2
A	1252	PHE	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	GLY	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
B	10	GLU	-	expression tag	UNP P0DTC2
B	11	THR	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	THR	-	expression tag	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
B	1237	GLN	-	expression tag	UNP P0DTC2
B	1238	ALA	-	expression tag	UNP P0DTC2
B	1239	TYR	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	ARG	-	expression tag	UNP P0DTC2
B	1242	LYS	-	expression tag	UNP P0DTC2
B	1243	ASP	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	GLU	-	expression tag	UNP P0DTC2
B	1246	TRP	-	expression tag	UNP P0DTC2
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
C	10	GLU	-	expression tag	UNP P0DTC2
C	11	THR	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	THR	-	expression tag	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	1212	GLY	-	expression tag	UNP P0DTC2
C	1213	SER	-	expression tag	UNP P0DTC2
C	1214	GLY	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	GLU	-	expression tag	UNP P0DTC2
C	1217	ASN	-	expression tag	UNP P0DTC2
C	1218	LEU	-	expression tag	UNP P0DTC2
C	1219	TYR	-	expression tag	UNP P0DTC2
C	1220	PHE	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLY	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	SER	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	TYR	-	expression tag	UNP P0DTC2
C	1229	ILE	-	expression tag	UNP P0DTC2
C	1230	PRO	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	ALA	-	expression tag	UNP P0DTC2
C	1233	PRO	-	expression tag	UNP P0DTC2
C	1234	ARG	-	expression tag	UNP P0DTC2
C	1235	ASP	-	expression tag	UNP P0DTC2
C	1236	GLY	-	expression tag	UNP P0DTC2
C	1237	GLN	-	expression tag	UNP P0DTC2
C	1238	ALA	-	expression tag	UNP P0DTC2
C	1239	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	ARG	-	expression tag	UNP P0DTC2
C	1242	LYS	-	expression tag	UNP P0DTC2
C	1243	ASP	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	GLU	-	expression tag	UNP P0DTC2
C	1246	TRP	-	expression tag	UNP P0DTC2
C	1247	VAL	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	LEU	-	expression tag	UNP P0DTC2
C	1250	SER	-	expression tag	UNP P0DTC2
C	1251	THR	-	expression tag	UNP P0DTC2
C	1252	PHE	-	expression tag	UNP P0DTC2
C	1253	LEU	-	expression tag	UNP P0DTC2
C	1254	GLY	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2

- 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
			Total	C	N	O		
2	D	2	28	16	2	10	0	0
2	E	2	28	16	2	10	0	0
2	F	2	28	16	2	10	0	0
2	G	2	28	16	2	10	0	0
2	H	2	28	16	2	10	0	0
2	I	2	28	16	2	10	0	0

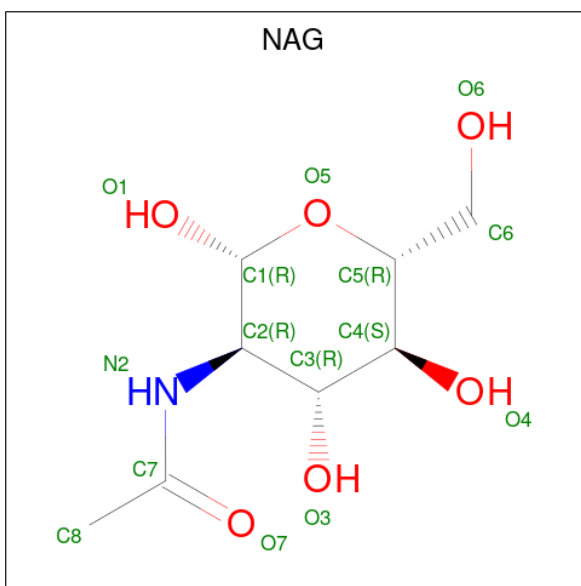
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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	J	2	Total 28	C 16	N 2	O 10	0	0
2	K	2	Total 28	C 16	N 2	O 10	0	0
2	L	2	Total 28	C 16	N 2	O 10	0	0
2	M	2	Total 28	C 16	N 2	O 10	0	0
2	N	2	Total 28	C 16	N 2	O 10	0	0
2	O	2	Total 28	C 16	N 2	O 10	0	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	Total 168	C 96	N 12	O 60	0
3	A	1	Total 168	C 96	N 12	O 60	0
3	A	1	Total 168	C 96	N 12	O 60	0
3	A	1	Total 168	C 96	N 12	O 60	0
3	A	1	Total 168	C 96	N 12	O 60	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	168	96	12	60	0
3	A	1	168	96	12	60	0
3	A	1	168	96	12	60	0
3	A	1	168	96	12	60	0
3	A	1	168	96	12	60	0
3	A	1	168	96	12	60	0
3	A	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	B	1	168	96	12	60	0
3	C	1	168	96	12	60	0
3	C	1	168	96	12	60	0

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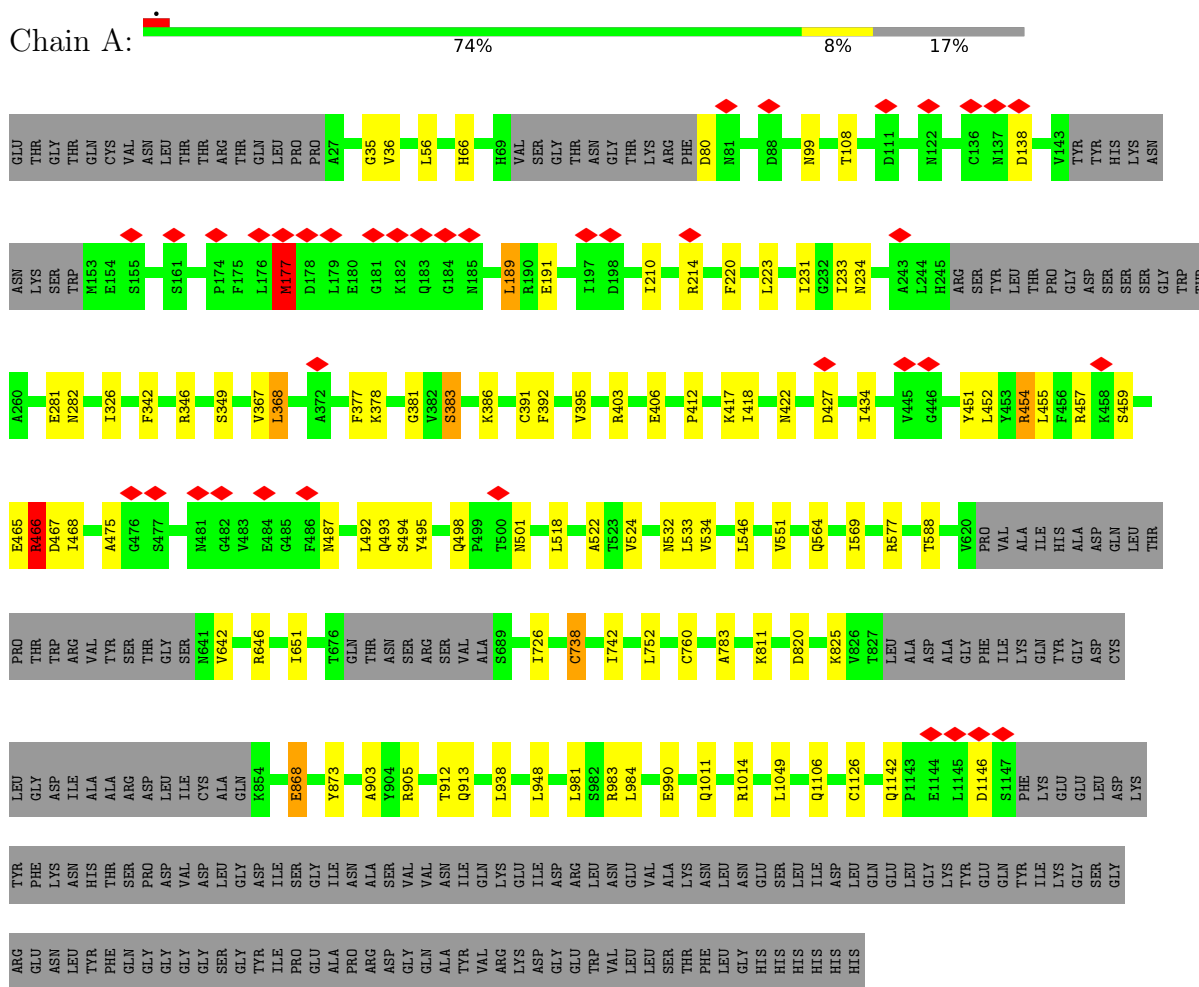
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0
3	C	1	Total 168	C 96	N 12	O 60	0

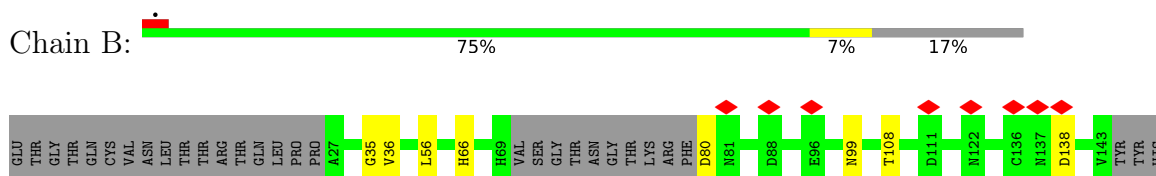
### 3 Residue-property plots

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





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

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

Chain D:  100%

WAG1  
WAG2

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

Chain E:  100%

WAG1  
WAG2

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

Chain F:  100%

WAG1  
WAG2

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

Chain G:  100%

WAG1  
WAG2

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

Chain H:  100%

WAG1  
WAG2

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

Chain I:  100%

WAG1  
WAG2

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

Chain J:  100%

MAG1  
MAG2

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

Chain K:  100%

MAG1  
MAG2

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

Chain L:  100%

MAG1  
MAG2

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

Chain M:  100%

MAG1  
MAG2

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

Chain N:  100%

MAG1  
MAG2

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

Chain O:  100%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	328188	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.189	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0222	Depositor
Map size (Å)	271.616, 271.616, 271.616	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.43	3/8218 (0.0%)	0.80	24/11177 (0.2%)
1	B	0.43	3/8218 (0.0%)	0.81	24/11177 (0.2%)
1	C	0.43	3/8218 (0.0%)	0.81	24/11177 (0.2%)
All	All	0.43	9/24654 (0.0%)	0.81	72/33531 (0.2%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	738	CYS	CB-SG	-6.22	1.71	1.82
1	A	738	CYS	CB-SG	-6.22	1.71	1.82
1	C	738	CYS	CB-SG	-6.22	1.71	1.82
1	C	760	CYS	CB-SG	-5.91	1.72	1.81
1	A	760	CYS	CB-SG	-5.88	1.72	1.81
1	B	760	CYS	CB-SG	-5.85	1.72	1.81
1	B	377	PHE	CD2-CE2	-5.31	1.28	1.39
1	C	377	PHE	CD2-CE2	-5.29	1.28	1.39
1	A	377	PHE	CD2-CE2	-5.27	1.28	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	MET	CB-CG-SD	11.49	146.88	112.40
1	B	177	MET	CB-CG-SD	11.49	146.87	112.40
1	C	177	MET	CB-CG-SD	11.49	146.87	112.40
1	B	466	ARG	CD-NE-CZ	10.40	138.16	123.60
1	C	466	ARG	CD-NE-CZ	10.40	138.16	123.60
1	A	466	ARG	CD-NE-CZ	10.38	138.13	123.60
1	A	738	CYS	CA-CB-SG	10.13	132.24	114.00
1	B	738	CYS	CA-CB-SG	10.11	132.19	114.00
1	C	738	CYS	CA-CB-SG	10.10	132.18	114.00
1	C	646	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	B	646	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	A	646	ARG	NE-CZ-NH1	-8.25	116.17	120.30
1	B	1126	CYS	CA-CB-SG	8.10	128.59	114.00
1	A	1126	CYS	CA-CB-SG	8.10	128.58	114.00
1	C	1126	CYS	CA-CB-SG	8.09	128.56	114.00
1	A	868	GLU	CA-CB-CG	8.08	131.17	113.40
1	B	868	GLU	CA-CB-CG	8.06	131.14	113.40
1	C	868	GLU	CA-CB-CG	8.05	131.12	113.40
1	C	378	LYS	CD-CE-NZ	7.61	129.19	111.70
1	A	378	LYS	CD-CE-NZ	7.60	129.18	111.70
1	B	378	LYS	CD-CE-NZ	7.59	129.15	111.70
1	B	466	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	455	LEU	CA-CB-CG	7.49	132.53	115.30
1	B	455	LEU	CA-CB-CG	7.47	132.49	115.30
1	C	466	ARG	NE-CZ-NH2	-7.47	116.57	120.30
1	C	455	LEU	CA-CB-CG	7.47	132.47	115.30
1	A	466	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	177	MET	CA-CB-CG	7.35	125.79	113.30
1	C	177	MET	CA-CB-CG	7.33	125.76	113.30
1	A	177	MET	CA-CB-CG	7.31	125.73	113.30
1	A	378	LYS	CB-CG-CD	7.15	130.18	111.60
1	B	378	LYS	CB-CG-CD	7.14	130.17	111.60
1	C	378	LYS	CB-CG-CD	7.14	130.16	111.60
1	C	377	PHE	CB-CG-CD1	6.41	125.29	120.80
1	C	646	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	B	377	PHE	CB-CG-CD1	6.36	125.25	120.80
1	B	377	PHE	CB-CG-CD2	-6.33	116.37	120.80
1	A	377	PHE	CB-CG-CD1	6.32	125.22	120.80
1	B	646	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	C	377	PHE	CB-CG-CD2	-6.31	116.38	120.80
1	A	377	PHE	CB-CG-CD2	-6.29	116.40	120.80
1	A	646	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	C	546	LEU	CB-CG-CD2	6.18	121.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	546	LEU	CB-CG-CD2	6.18	121.50	111.00
1	A	546	LEU	CB-CG-CD2	6.18	121.50	111.00
1	B	177	MET	CG-SD-CE	6.07	109.92	100.20
1	C	177	MET	CG-SD-CE	6.07	109.91	100.20
1	A	177	MET	CG-SD-CE	6.07	109.90	100.20
1	C	738	CYS	CB-CA-C	-5.94	98.52	110.40
1	B	738	CYS	CB-CA-C	-5.92	98.55	110.40
1	A	738	CYS	CB-CA-C	-5.92	98.56	110.40
1	C	378	LYS	CB-CA-C	5.77	121.94	110.40
1	B	378	LYS	CB-CA-C	5.75	121.91	110.40
1	A	378	LYS	CB-CA-C	5.74	121.88	110.40
1	C	454	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	455	LEU	CB-CG-CD2	5.61	120.53	111.00
1	C	455	LEU	CB-CG-CD2	5.61	120.53	111.00
1	B	455	LEU	CB-CG-CD2	5.59	120.50	111.00
1	C	189	LEU	CB-CG-CD2	5.52	120.39	111.00
1	A	189	LEU	CB-CG-CD2	5.51	120.36	111.00
1	B	189	LEU	CB-CG-CD2	5.51	120.36	111.00
1	B	454	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	454	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	378	LYS	CA-CB-CG	5.34	125.15	113.40
1	B	378	LYS	CA-CB-CG	5.33	125.12	113.40
1	C	378	LYS	CA-CB-CG	5.32	125.10	113.40
1	C	417	LYS	CD-CE-NZ	-5.15	99.86	111.70
1	B	417	LYS	CD-CE-NZ	-5.14	99.89	111.70
1	A	417	LYS	CD-CE-NZ	-5.13	99.89	111.70
1	C	368	LEU	CA-CB-CG	5.05	126.93	115.30
1	A	368	LEU	CA-CB-CG	5.04	126.90	115.30
1	B	368	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	466	ARG	Sidechain
1	B	466	ARG	Sidechain
1	C	466	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8039	0	7831	57	0
1	B	8039	0	7831	55	0
1	C	8039	0	7831	55	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
3	A	168	0	156	3	0
3	B	168	0	156	3	0
3	C	168	0	156	2	0
All	All	24957	0	24261	160	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.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:VAL:HG23	1:B:524:VAL:HG11	1.70	0.73
1:B:66:HIS:O	1:B:80:ASP:N	2.22	0.72
1:C:395:VAL:HG23	1:C:524:VAL:HG11	1.70	0.72
1:A:395:VAL:HG23	1:A:524:VAL:HG11	1.70	0.72
1:C:66:HIS:O	1:C:80:ASP:N	2.22	0.71
1:A:66:HIS:O	1:A:80:ASP:N	2.22	0.71
1:B:912:THR:OG1	1:B:1106:GLN:NE2	2.25	0.70
1:A:912:THR:OG1	1:A:1106:GLN:NE2	2.25	0.69
1:C:912:THR:OG1	1:C:1106:GLN:NE2	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:ARG:NH2	1:C:467:ASP:O	2.28	0.67
1:B:454:ARG:NH2	1:B:467:ASP:O	2.28	0.66
1:A:454:ARG:NH2	1:A:467:ASP:O	2.28	0.66
1:B:1142:GLN:NE2	1:B:1146:ASP:OD2	2.30	0.65
1:C:1142:GLN:NE2	1:C:1146:ASP:OD2	2.30	0.64
1:B:282:ASN:OD1	3:B:1304:NAG:N2	2.30	0.64
1:A:282:ASN:OD1	3:A:1304:NAG:N2	2.30	0.64
1:C:349:SER:OG	1:C:452:LEU:O	2.15	0.64
1:B:349:SER:OG	1:B:452:LEU:O	2.15	0.64
1:C:282:ASN:OD1	3:C:1304:NAG:N2	2.31	0.64
1:A:1142:GLN:NE2	1:A:1146:ASP:OD2	2.30	0.64
1:A:349:SER:OG	1:A:452:LEU:O	2.15	0.63
1:B:983:ARG:NH1	1:C:381:GLY:O	2.32	0.63
1:A:381:GLY:O	1:C:983:ARG:NH1	2.32	0.62
1:B:406:GLU:N	1:B:406:GLU:OE2	2.33	0.62
1:A:406:GLU:N	1:A:406:GLU:OE2	2.33	0.62
1:A:983:ARG:NH1	1:B:381:GLY:O	2.34	0.61
1:C:108:THR:OG1	1:C:234:ASN:O	2.19	0.61
1:C:406:GLU:N	1:C:406:GLU:OE2	2.33	0.61
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.33	0.61
1:B:108:THR:OG1	1:B:234:ASN:O	2.19	0.60
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.33	0.60
1:A:383:SER:HB3	1:C:984:LEU:HA	1.84	0.60
1:A:108:THR:OG1	1:A:234:ASN:O	2.19	0.60
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.33	0.59
1:C:1011:GLN:OE1	1:C:1014:ARG:NH1	2.37	0.58
1:A:903:ALA:HB1	1:A:913:GLN:HB2	1.85	0.58
1:B:1011:GLN:OE1	1:B:1014:ARG:NH1	2.37	0.58
1:C:903:ALA:HB1	1:C:913:GLN:HB2	1.85	0.57
1:A:984:LEU:HA	1:B:383:SER:HB3	1.85	0.57
1:A:1011:GLN:OE1	1:A:1014:ARG:NH1	2.37	0.57
1:B:903:ALA:HB1	1:B:913:GLN:HB2	1.85	0.56
1:B:984:LEU:HA	1:C:383:SER:HB3	1.86	0.56
1:A:403:ARG:NE	1:A:406:GLU:OE1	2.39	0.54
1:A:457:ARG:NH1	1:A:459:SER:OG	2.41	0.54
1:B:493:GLN:NE2	1:B:494:SER:O	2.41	0.53
1:B:642:VAL:HG12	1:B:651:ILE:CD1	2.39	0.53
1:C:493:GLN:NE2	1:C:494:SER:O	2.41	0.53
1:C:642:VAL:HG12	1:C:651:ILE:CD1	2.39	0.53
1:B:457:ARG:NH1	1:B:459:SER:OG	2.41	0.53
1:C:403:ARG:NE	1:C:406:GLU:OE1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ILE:HD11	1:B:534:VAL:HG22	1.91	0.53
1:A:326:ILE:HD11	1:A:534:VAL:HG22	1.91	0.53
1:C:457:ARG:NH1	1:C:459:SER:OG	2.41	0.53
1:A:493:GLN:NE2	1:A:494:SER:O	2.41	0.52
1:A:564:GLN:NE2	1:A:577:ARG:O	2.43	0.52
1:A:642:VAL:HG12	1:A:651:ILE:CD1	2.39	0.52
1:B:367:VAL:HG23	1:B:368:LEU:HD12	1.92	0.52
1:C:326:ILE:HD11	1:C:534:VAL:HG22	1.91	0.52
1:C:367:VAL:HG23	1:C:368:LEU:HD12	1.92	0.52
1:B:403:ARG:NE	1:B:406:GLU:OE1	2.39	0.52
1:C:564:GLN:NE2	1:C:577:ARG:O	2.43	0.52
1:B:564:GLN:NE2	1:B:577:ARG:O	2.43	0.52
1:B:200:TYR:HH	1:C:396:TYR:HE2	1.58	0.51
1:A:342:PHE:HE1	1:A:434:ILE:HG21	1.75	0.51
1:B:342:PHE:HE1	1:B:434:ILE:HG21	1.75	0.51
1:A:367:VAL:HG23	1:A:368:LEU:HD12	1.92	0.51
1:C:342:PHE:HE1	1:C:434:ILE:HG21	1.75	0.51
1:C:551:VAL:HG12	1:C:588:THR:O	2.11	0.51
1:B:551:VAL:HG12	1:B:588:THR:O	2.11	0.51
1:B:983:ARG:HG3	1:B:984:LEU:HD12	1.93	0.51
1:A:551:VAL:HG12	1:A:588:THR:O	2.11	0.50
1:A:386:LYS:NZ	1:C:981:LEU:O	2.45	0.50
1:A:983:ARG:HG3	1:A:984:LEU:HD12	1.93	0.50
1:B:981:LEU:O	1:C:386:LYS:NZ	2.45	0.50
1:B:36:VAL:HG11	1:B:220:PHE:CE2	2.47	0.49
1:C:983:ARG:HG3	1:C:984:LEU:HD12	1.93	0.49
1:A:981:LEU:O	1:B:386:LYS:NZ	2.46	0.49
1:B:726:ILE:HG22	1:B:948:LEU:HD13	1.95	0.49
1:C:346:ARG:NH2	1:C:451:TYR:OH	2.46	0.49
1:C:36:VAL:HG11	1:C:220:PHE:CE2	2.47	0.48
1:A:346:ARG:NH2	1:A:451:TYR:OH	2.46	0.48
1:B:346:ARG:NH2	1:B:451:TYR:OH	2.46	0.48
1:A:189:LEU:HB2	1:A:210:ILE:HD13	1.95	0.48
1:B:189:LEU:HB2	1:B:210:ILE:HD13	1.95	0.48
1:A:726:ILE:HG22	1:A:948:LEU:HD13	1.95	0.48
1:C:189:LEU:HB2	1:C:210:ILE:HD13	1.95	0.48
1:A:36:VAL:HG11	1:A:220:PHE:CE2	2.47	0.48
1:C:726:ILE:HG22	1:C:948:LEU:HD13	1.95	0.48
1:B:524:VAL:HG13	1:B:524:VAL:O	2.14	0.48
1:C:498:GLN:OE1	1:C:501:ASN:ND2	2.45	0.47
1:C:524:VAL:O	1:C:524:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLN:OE1	1:A:501:ASN:ND2	2.45	0.47
1:A:35:GLY:HA3	1:A:56:LEU:HB3	1.97	0.47
1:B:35:GLY:HA3	1:B:56:LEU:HB3	1.97	0.47
1:C:518:LEU:HD11	1:C:522:ALA:HB2	1.97	0.46
1:A:524:VAL:HG13	1:A:524:VAL:O	2.14	0.46
1:B:465:GLU:N	1:B:465:GLU:OE1	2.49	0.46
1:C:465:GLU:OE1	1:C:465:GLU:N	2.48	0.46
1:C:35:GLY:HA3	1:C:56:LEU:HB3	1.97	0.46
1:B:518:LEU:HD11	1:B:522:ALA:HB2	1.97	0.46
1:A:642:VAL:HG12	1:A:651:ILE:HD12	1.98	0.45
1:B:642:VAL:HG12	1:B:651:ILE:HD12	1.98	0.45
1:A:465:GLU:N	1:A:465:GLU:OE1	2.48	0.45
1:C:452:LEU:HB3	1:C:492:LEU:HD12	1.98	0.45
1:C:642:VAL:HG12	1:C:651:ILE:HD12	1.98	0.45
1:C:825:LYS:NZ	1:C:938:LEU:O	2.42	0.45
1:A:452:LEU:HB3	1:A:492:LEU:HD12	1.98	0.45
3:B:1308:NAG:H83	3:B:1308:NAG:H3	1.99	0.45
3:A:1308:NAG:H83	3:A:1308:NAG:H3	1.99	0.45
1:A:518:LEU:HD11	1:A:522:ALA:HB2	1.97	0.45
1:A:391:CYS:SG	1:A:392:PHE:N	2.90	0.45
1:B:391:CYS:SG	1:B:522:ALA:HB1	2.57	0.45
3:C:1308:NAG:H83	3:C:1308:NAG:H3	1.99	0.44
1:A:138:ASP:N	1:A:138:ASP:OD1	2.51	0.44
1:B:452:LEU:HB3	1:B:492:LEU:HD12	1.98	0.44
1:C:391:CYS:SG	1:C:392:PHE:N	2.90	0.44
1:A:825:LYS:NZ	1:A:938:LEU:O	2.42	0.44
1:B:191:GLU:HB2	1:B:223:LEU:HD21	2.00	0.44
1:A:391:CYS:SG	1:A:522:ALA:HB1	2.57	0.43
1:A:466:ARG:HG2	1:A:468:ILE:HG23	2.00	0.43
1:B:391:CYS:SG	1:B:392:PHE:N	2.90	0.43
1:C:138:ASP:N	1:C:138:ASP:OD1	2.51	0.43
1:C:391:CYS:SG	1:C:522:ALA:HB1	2.57	0.43
1:C:466:ARG:HG2	1:C:468:ILE:HG23	2.00	0.43
1:B:99:ASN:ND2	1:B:177:MET:HG3	2.34	0.43
1:B:138:ASP:N	1:B:138:ASP:OD1	2.51	0.43
1:C:99:ASN:ND2	1:C:177:MET:HG3	2.34	0.43
1:C:783:ALA:HB2	1:C:873:TYR:HE2	1.84	0.43
1:C:231:ILE:HD12	1:C:233:ILE:HG12	2.00	0.43
1:A:99:ASN:ND2	1:A:177:MET:HG3	2.34	0.43
1:A:494:SER:OG	1:A:495:TYR:N	2.52	0.43
1:A:738:CYS:HB3	1:A:742:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:ALA:HB2	1:B:873:TYR:HE2	1.84	0.43
1:A:231:ILE:HD12	1:A:233:ILE:HG12	2.00	0.42
1:B:494:SER:OG	1:B:495:TYR:N	2.52	0.42
1:B:825:LYS:NZ	1:B:938:LEU:O	2.42	0.42
1:A:191:GLU:HB2	1:A:223:LEU:HD21	2.00	0.42
1:B:231:ILE:HD12	1:B:233:ILE:HG12	2.00	0.42
1:B:466:ARG:HG2	1:B:468:ILE:HG23	2.00	0.42
1:C:494:SER:OG	1:C:495:TYR:N	2.52	0.42
1:B:738:CYS:HB3	1:B:742:ILE:HD12	2.01	0.42
1:C:191:GLU:HB2	1:C:223:LEU:HD21	2.00	0.42
1:A:418:ILE:HG23	1:A:422:ASN:OD1	2.20	0.42
1:C:418:ILE:HG23	1:C:422:ASN:OD1	2.20	0.42
1:A:281:GLU:OE2	3:A:1304:NAG:N2	2.48	0.41
1:A:752:LEU:HD11	1:A:990:GLU:OE1	2.20	0.41
1:B:418:ILE:HG23	1:B:422:ASN:OD1	2.20	0.41
1:A:783:ALA:HB2	1:A:873:TYR:HE2	1.84	0.41
1:B:281:GLU:OE2	3:B:1304:NAG:N2	2.48	0.41
1:A:475:ALA:HB3	1:A:487:ASN:HA	2.03	0.41
1:C:752:LEU:HD11	1:C:990:GLU:OE1	2.20	0.41
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.47	0.41
1:B:498:GLN:OE1	1:B:501:ASN:ND2	2.45	0.41
1:B:752:LEU:HD11	1:B:990:GLU:OE1	2.20	0.41
1:C:738:CYS:HB3	1:C:742:ILE:HD12	2.01	0.41
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.51	0.41
1:B:412:PRO:HB3	1:B:427:ASP:HA	2.03	0.41
1:A:532:ASN:OD1	1:A:533:LEU:N	2.54	0.41
1:C:412:PRO:HB3	1:C:427:ASP:HA	2.03	0.41
1:A:412:PRO:HB3	1:A:427:ASP:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

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

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1016/1247 (82%)	980 (96%)	36 (4%)	0	100	100
1	B	1016/1247 (82%)	980 (96%)	36 (4%)	0	100	100
1	C	1016/1247 (82%)	980 (96%)	36 (4%)	0	100	100
All	All	3048/3741 (82%)	2940 (96%)	108 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	898/1081 (83%)	893 (99%)	5 (1%)	86	95
1	B	898/1081 (83%)	893 (99%)	5 (1%)	86	95
1	C	898/1081 (83%)	893 (99%)	5 (1%)	86	95
All	All	2694/3243 (83%)	2679 (99%)	15 (1%)	86	95

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	MET
1	A	214	ARG
1	A	383	SER
1	A	569	ILE
1	A	868	GLU
1	B	177	MET
1	B	214	ARG
1	B	383	SER
1	B	569	ILE
1	B	868	GLU
1	C	177	MET
1	C	214	ARG
1	C	383	SER
1	C	569	ILE
1	C	868	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1106	GLN
1	B	1106	GLN
1	C	1106	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

24 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	D	1	1,2	14,14,15	0.18	0	17,19,21	0.57	0
2	NAG	D	2	2	14,14,15	0.17	0	17,19,21	0.60	0
2	NAG	E	1	1,2	14,14,15	0.16	0	17,19,21	0.65	0
2	NAG	E	2	2	14,14,15	0.17	0	17,19,21	0.57	0
2	NAG	F	1	1,2	14,14,15	0.41	0	17,19,21	0.58	0
2	NAG	F	2	2	14,14,15	0.19	0	17,19,21	0.58	0
2	NAG	G	1	1,2	14,14,15	0.26	0	17,19,21	0.59	0
2	NAG	G	2	2	14,14,15	0.18	0	17,19,21	0.59	0
2	NAG	H	1	1,2	14,14,15	0.18	0	17,19,21	0.58	0
2	NAG	H	2	2	14,14,15	0.17	0	17,19,21	0.61	0
2	NAG	I	1	1,2	14,14,15	0.17	0	17,19,21	0.64	0
2	NAG	I	2	2	14,14,15	0.16	0	17,19,21	0.56	0
2	NAG	J	1	1,2	14,14,15	0.40	0	17,19,21	0.57	0
2	NAG	J	2	2	14,14,15	0.22	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	K	1	1,2	14,14,15	0.24	0	17,19,21	0.59	0
2	NAG	K	2	2	14,14,15	0.18	0	17,19,21	0.60	0
2	NAG	L	1	1,2	14,14,15	0.16	0	17,19,21	0.57	0
2	NAG	L	2	2	14,14,15	0.16	0	17,19,21	0.61	0
2	NAG	M	1	1,2	14,14,15	0.16	0	17,19,21	0.64	0
2	NAG	M	2	2	14,14,15	0.16	0	17,19,21	0.56	0
2	NAG	N	1	1,2	14,14,15	0.39	0	17,19,21	0.57	0
2	NAG	N	2	2	14,14,15	0.22	0	17,19,21	0.58	0
2	NAG	O	1	1,2	14,14,15	0.23	0	17,19,21	0.59	0
2	NAG	O	2	2	14,14,15	0.18	0	17,19,21	0.59	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

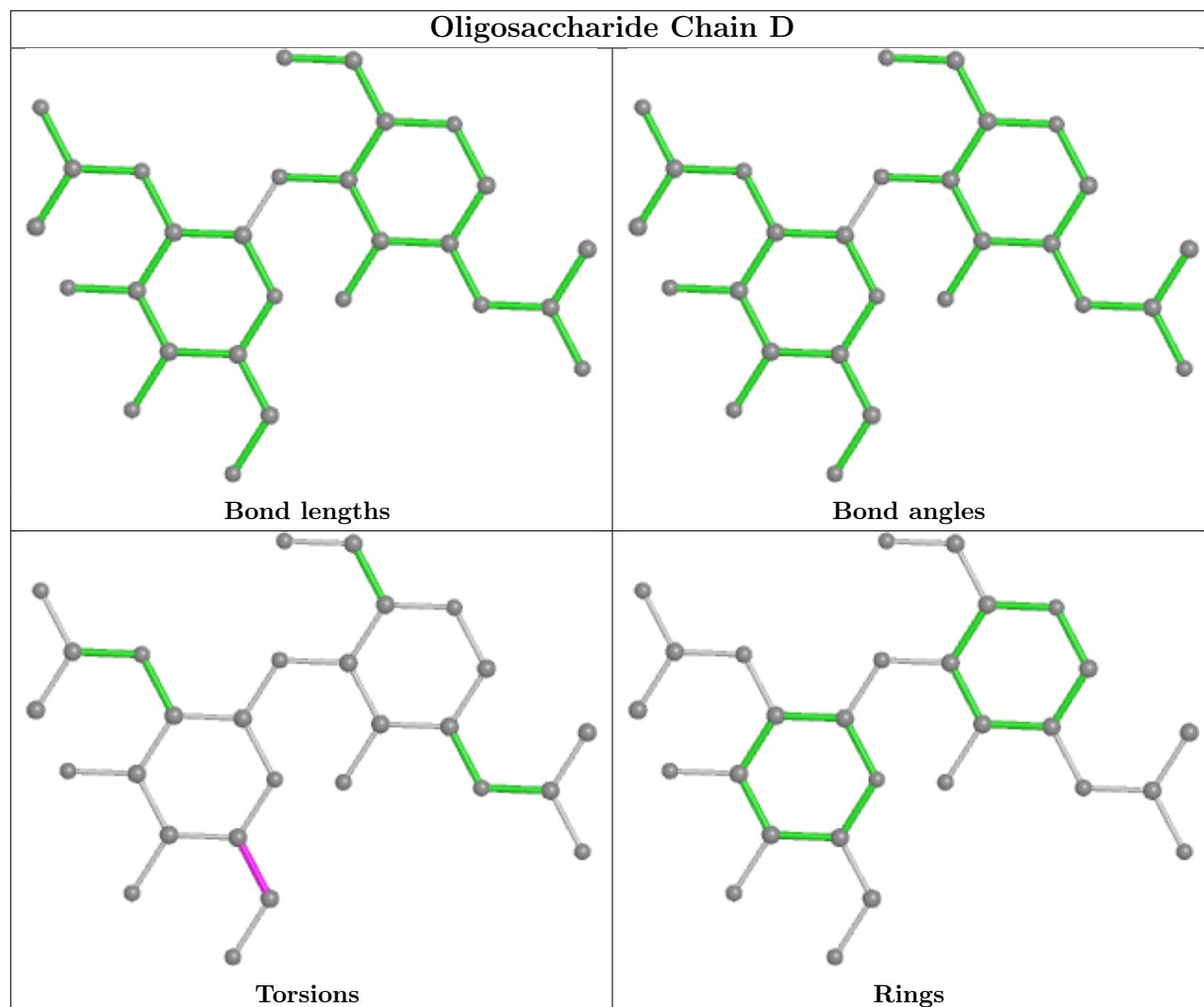
All (21) torsion outliers are listed below:

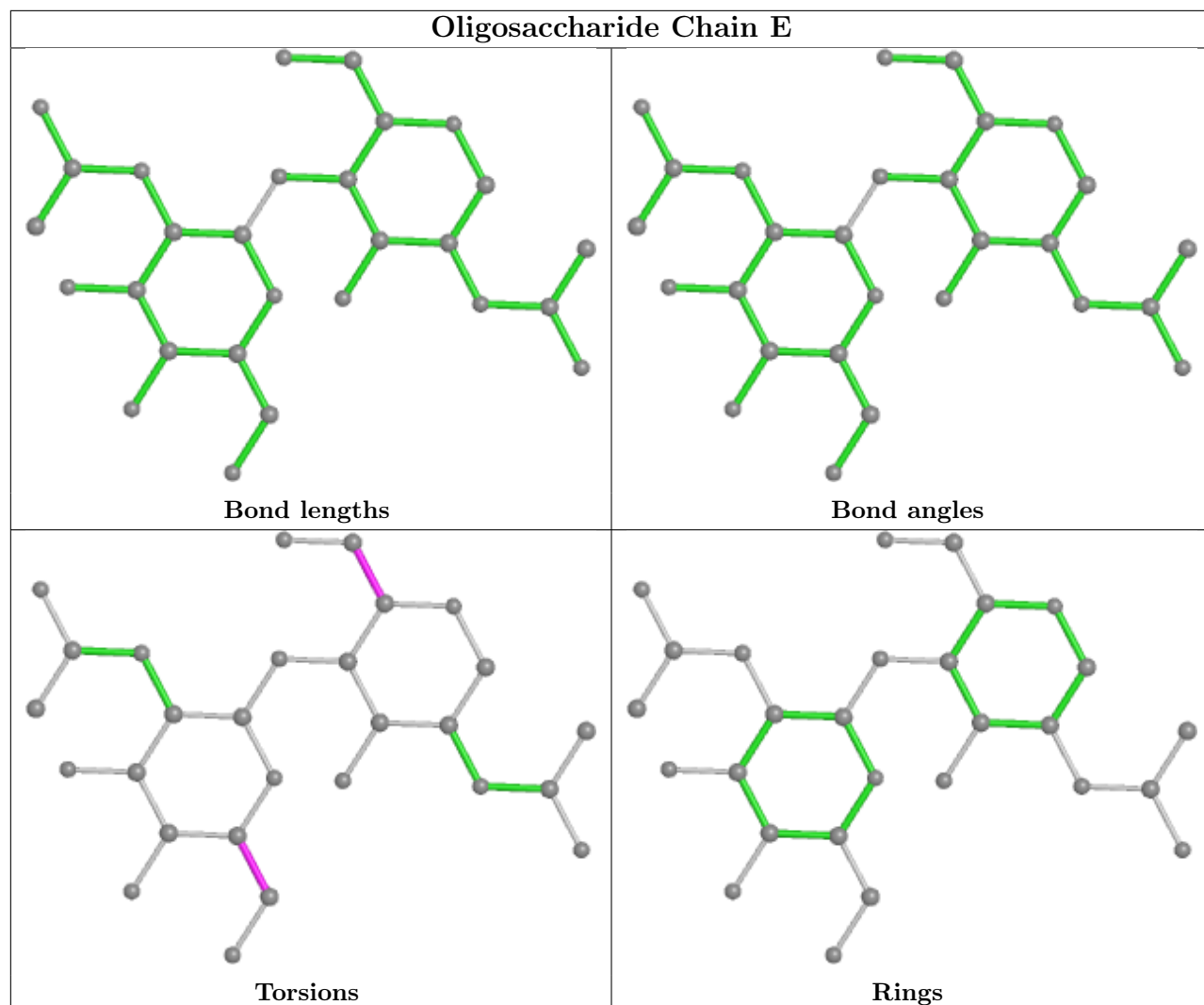
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6

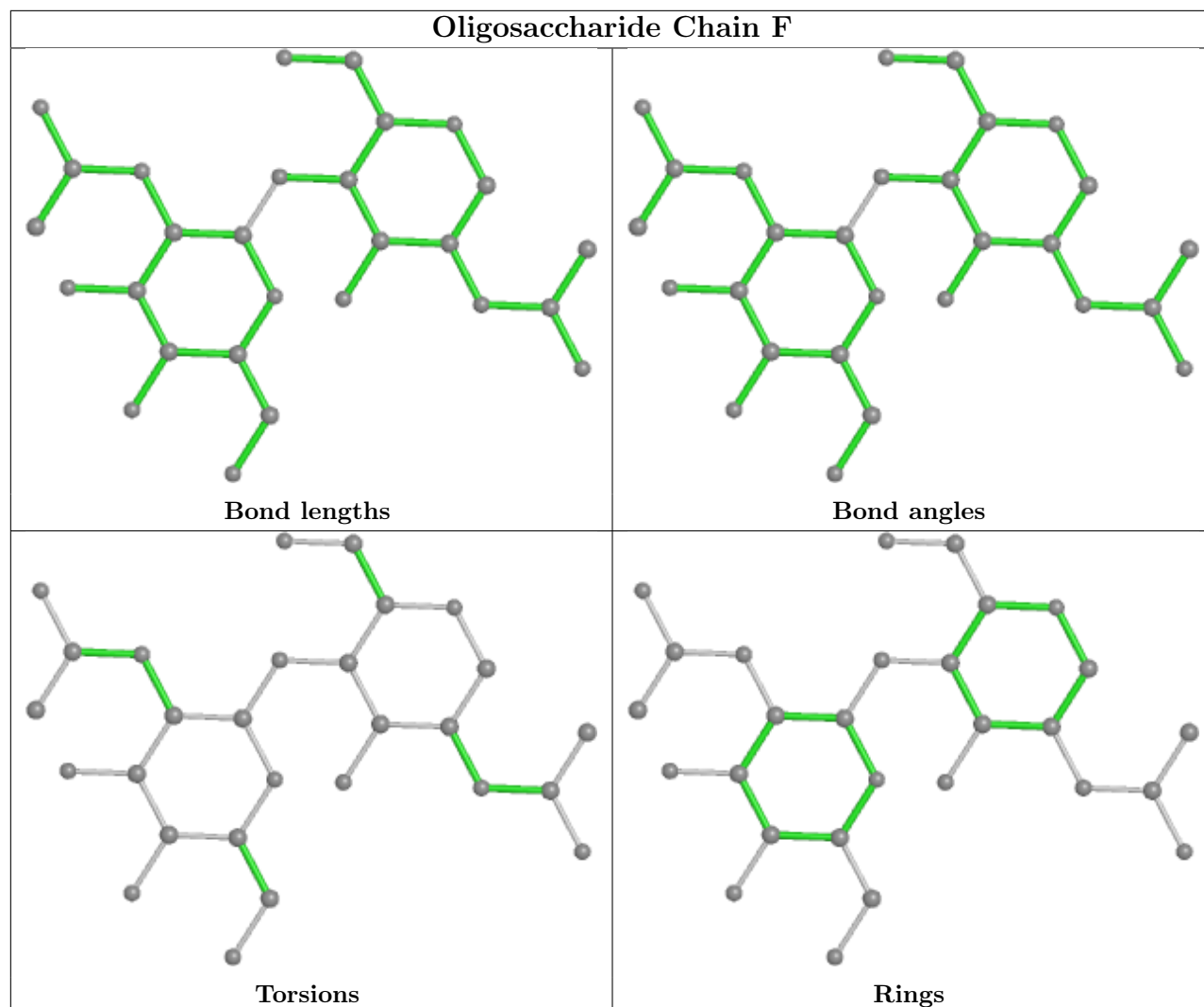
There are no ring outliers.

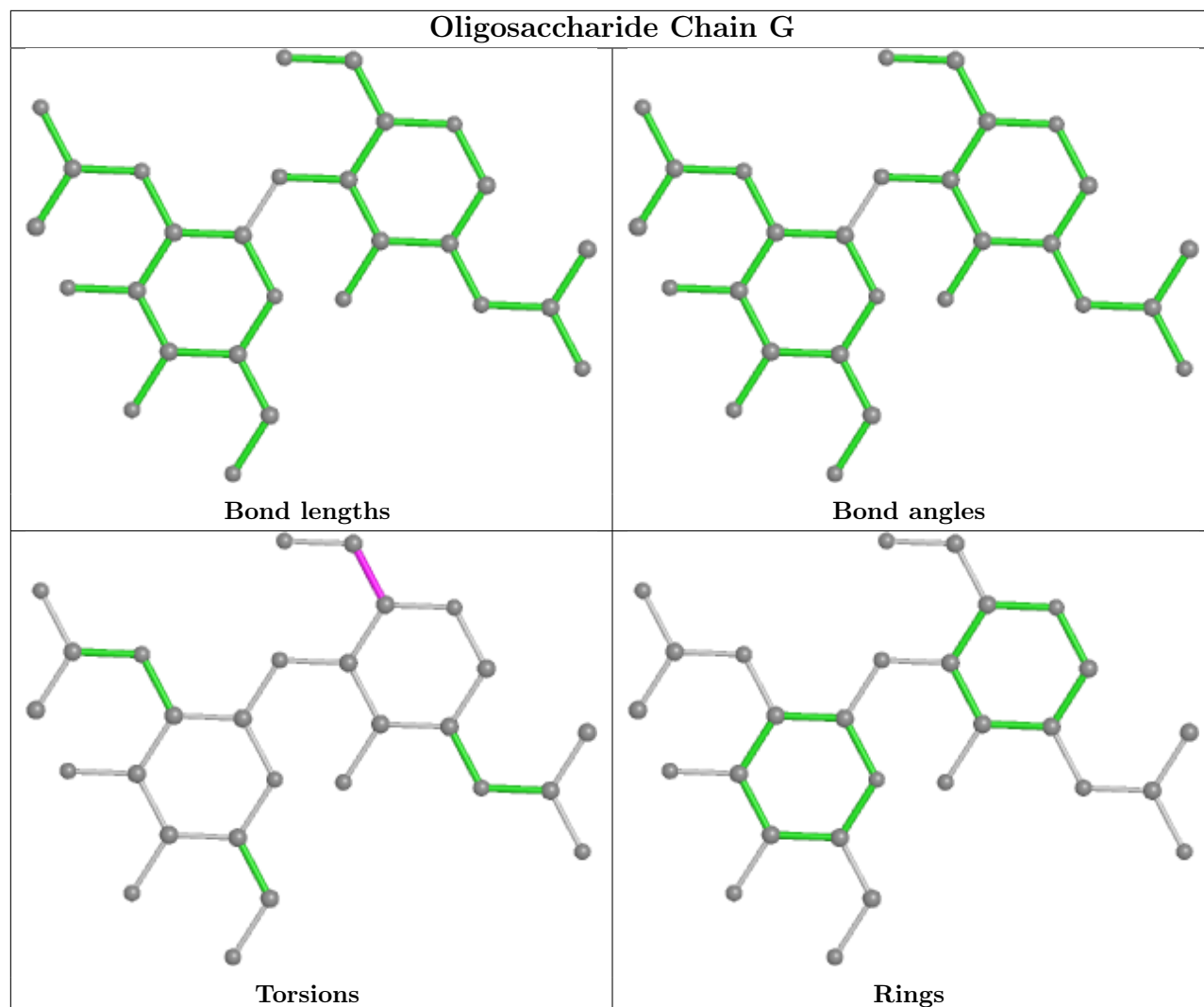
No monomer is involved in short contacts.

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

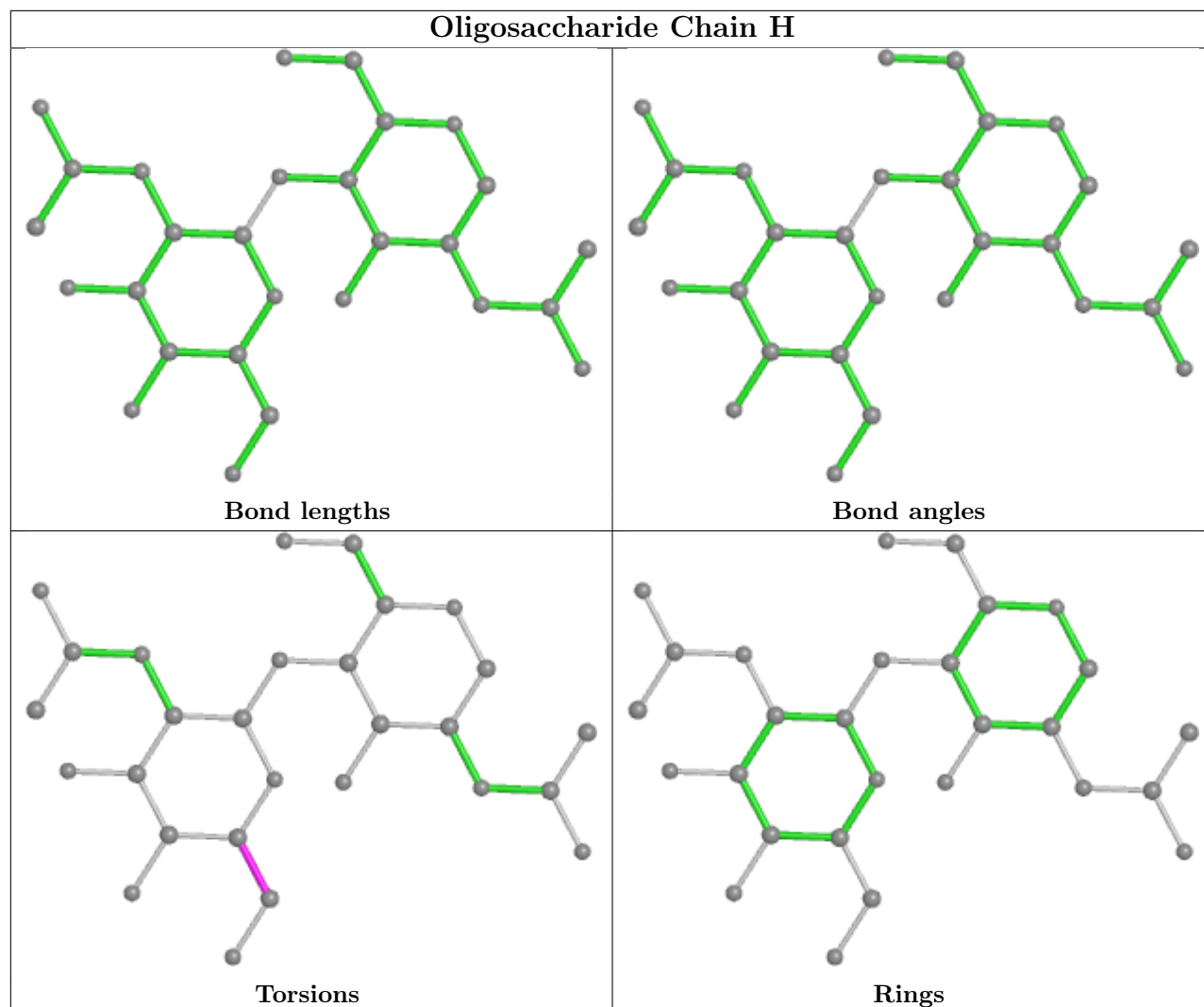


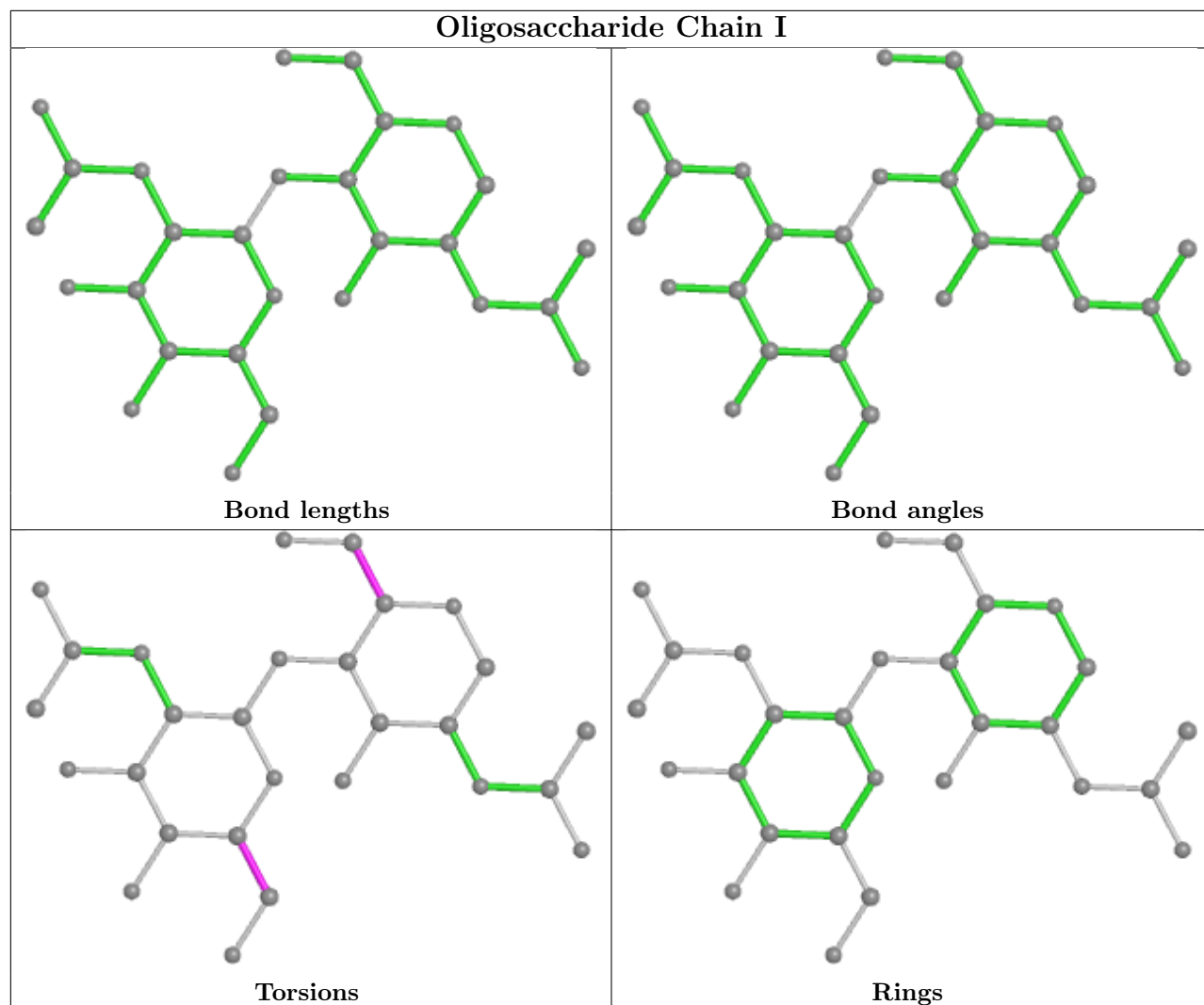


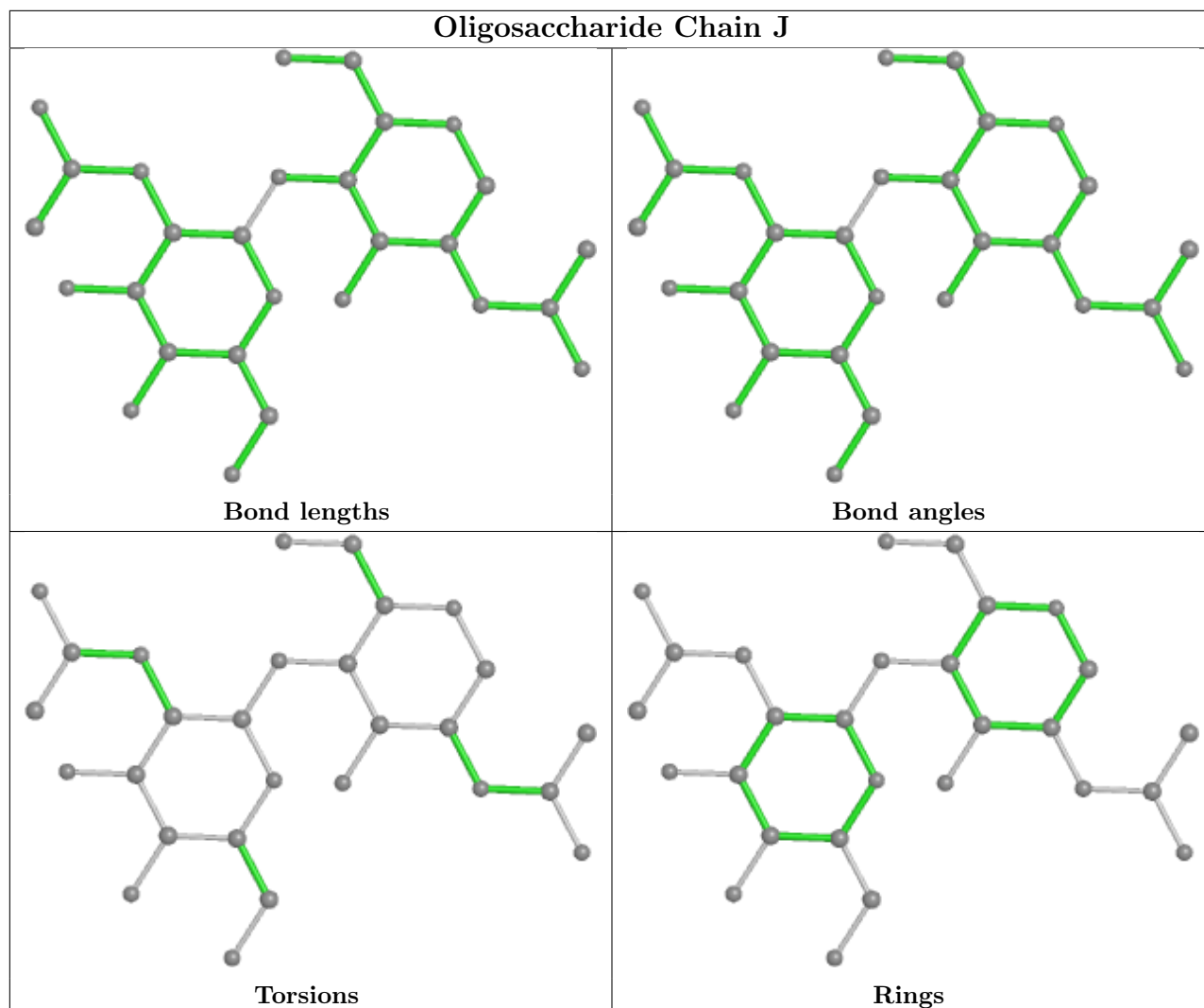


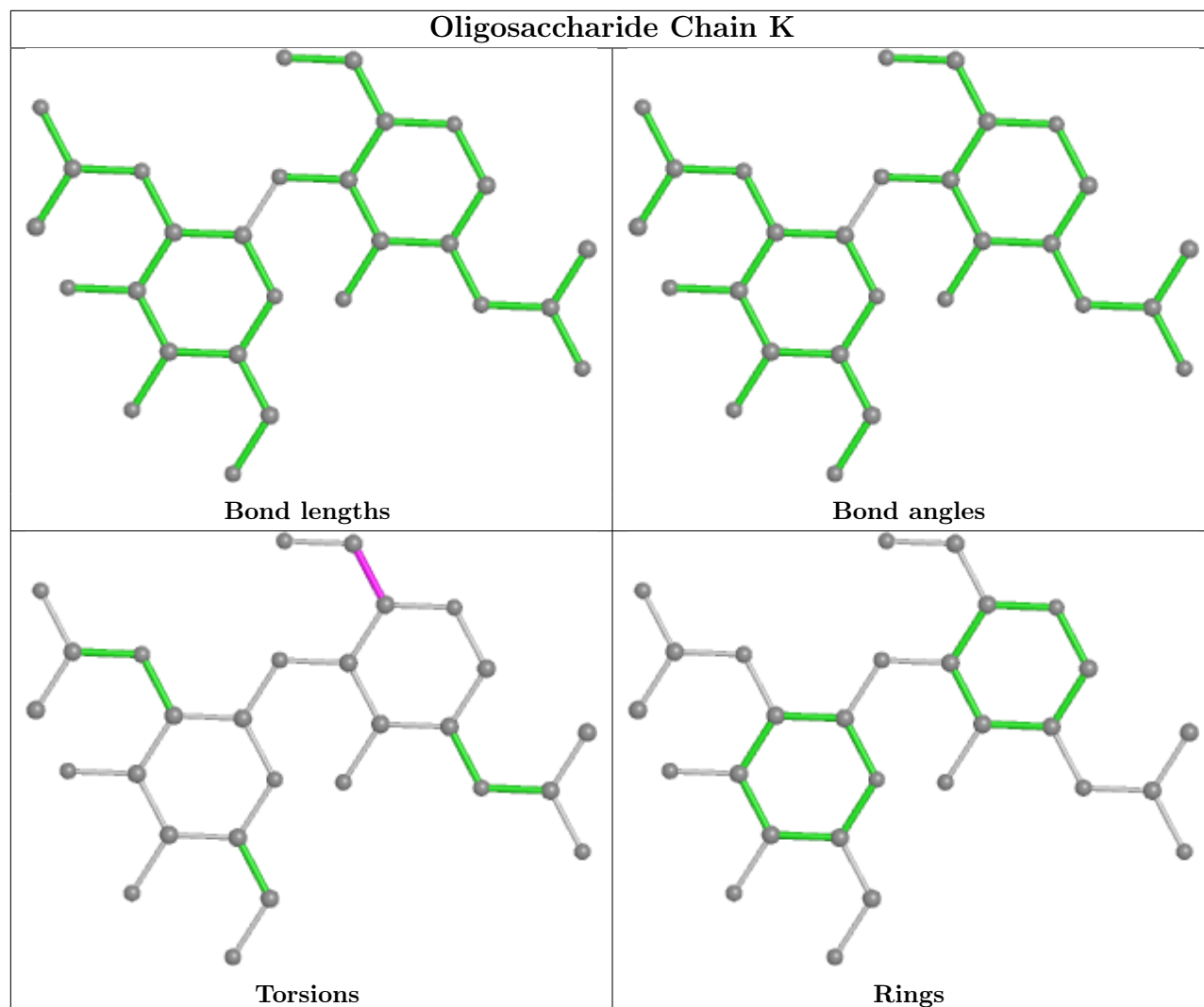


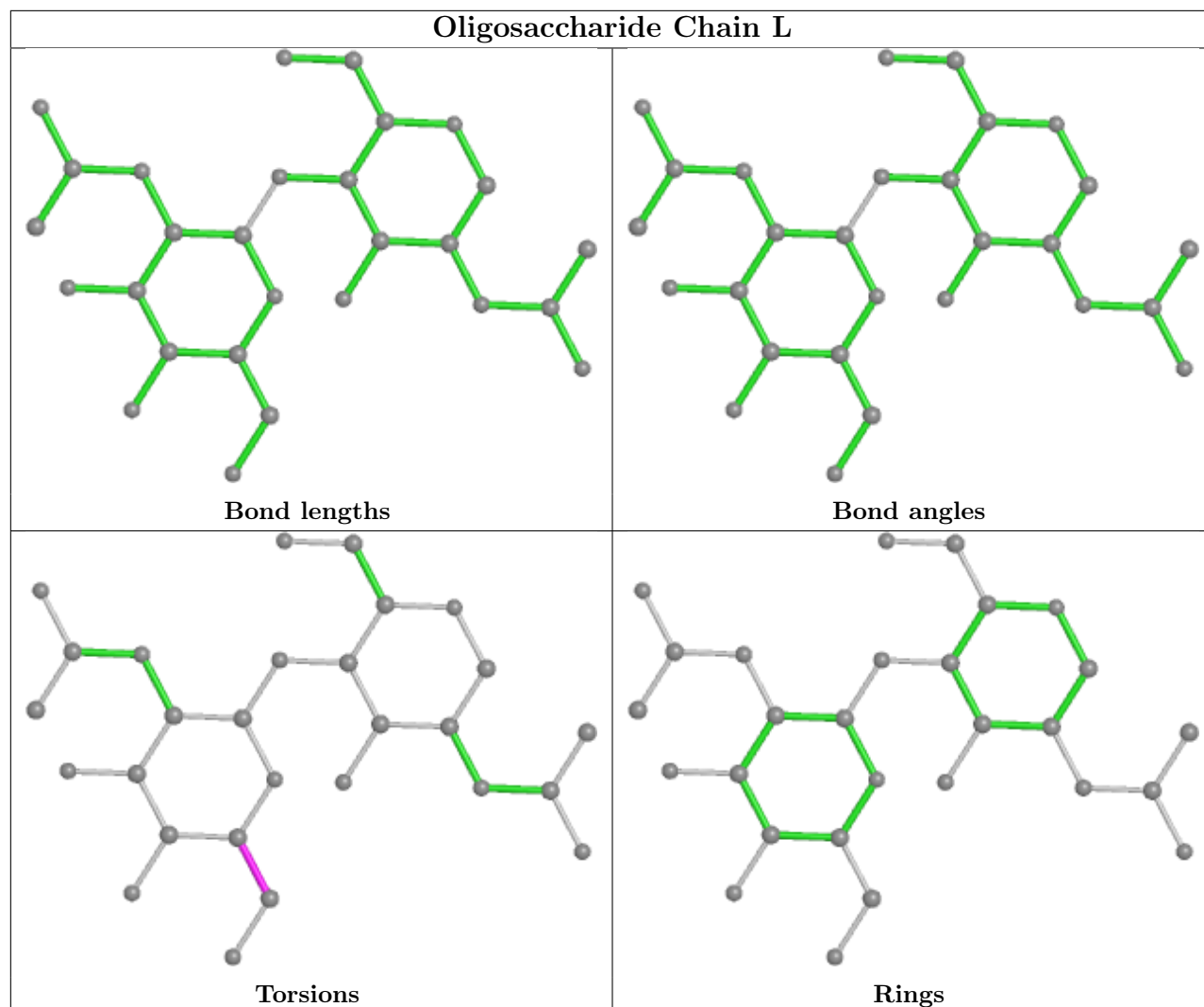


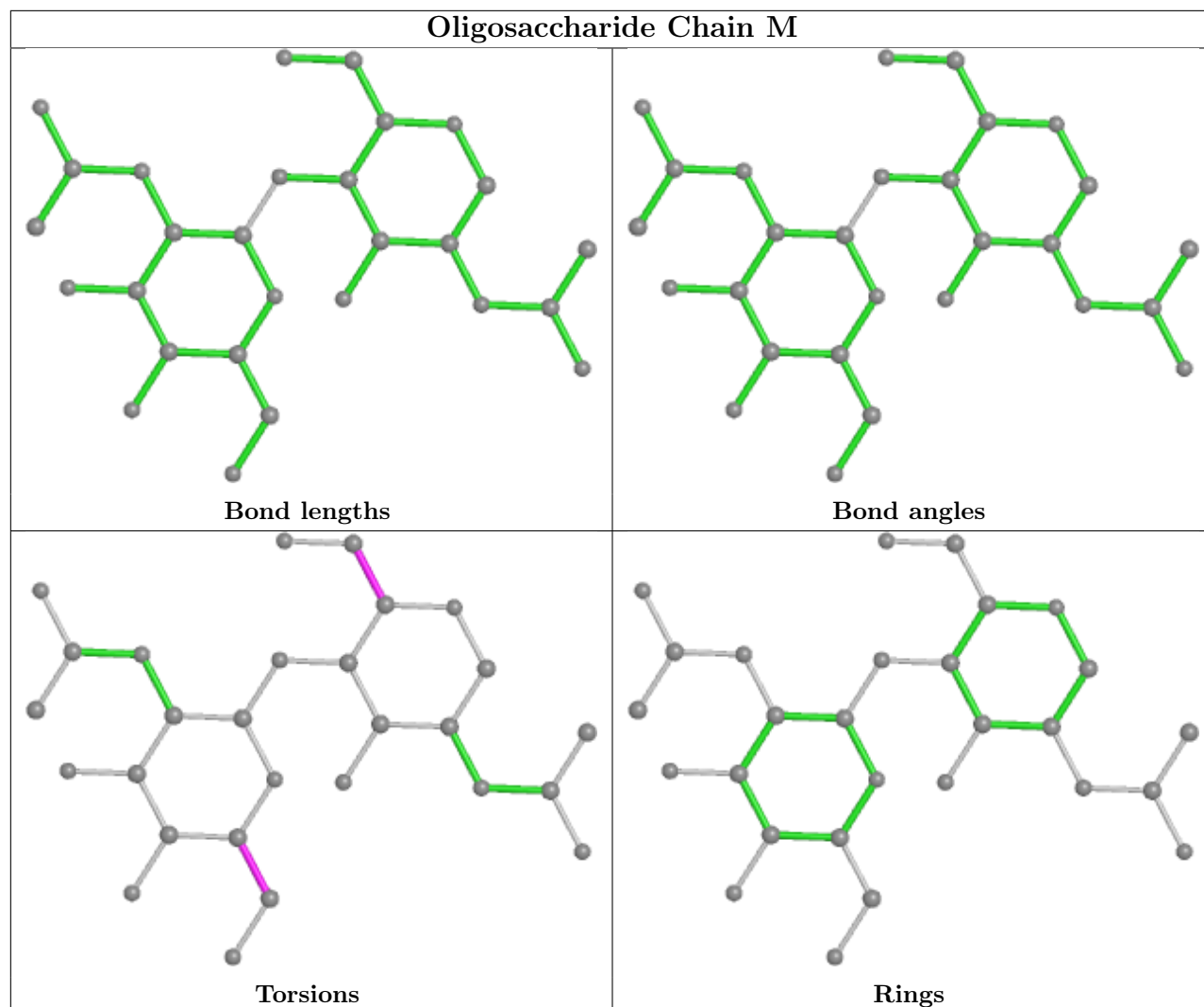


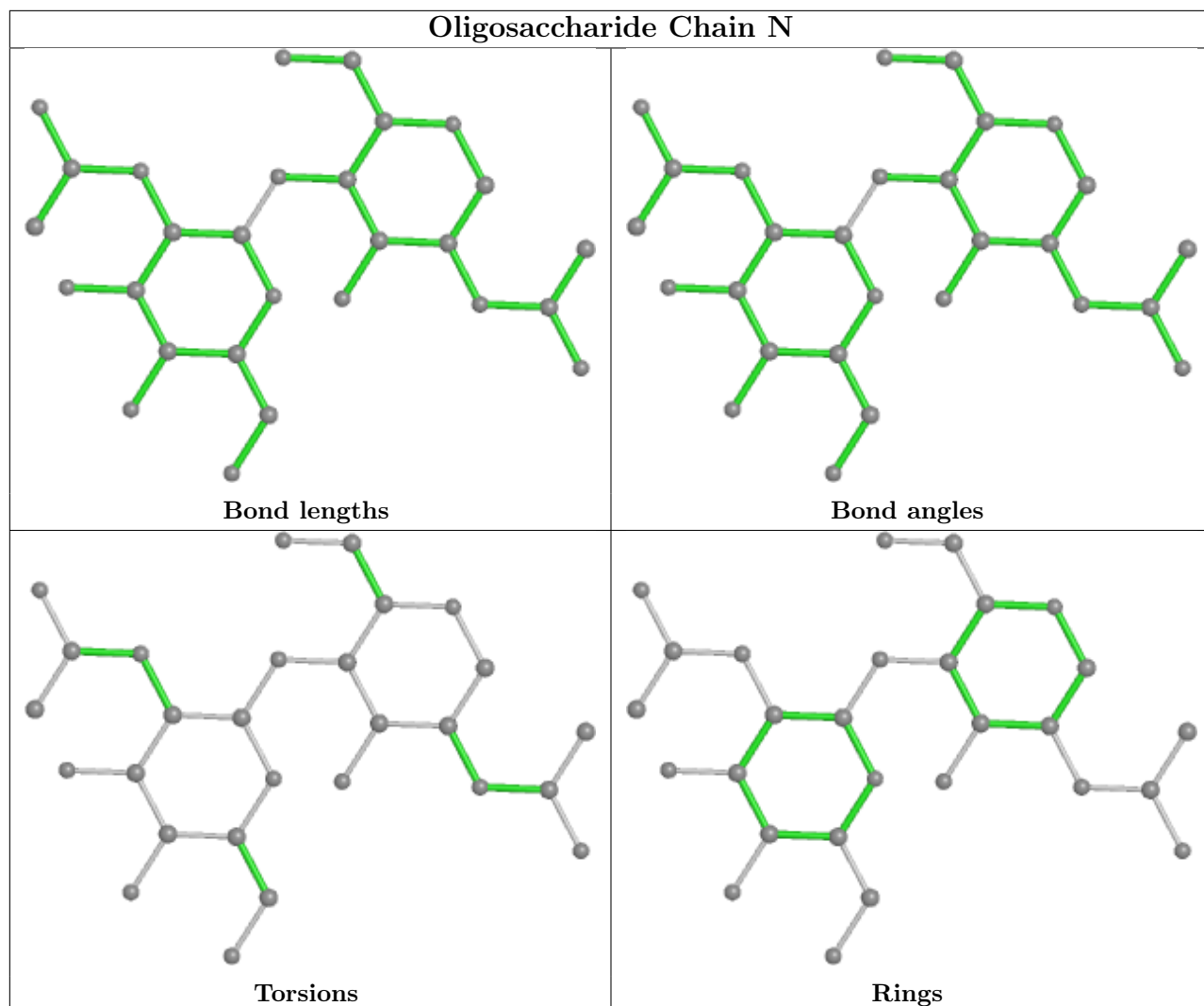


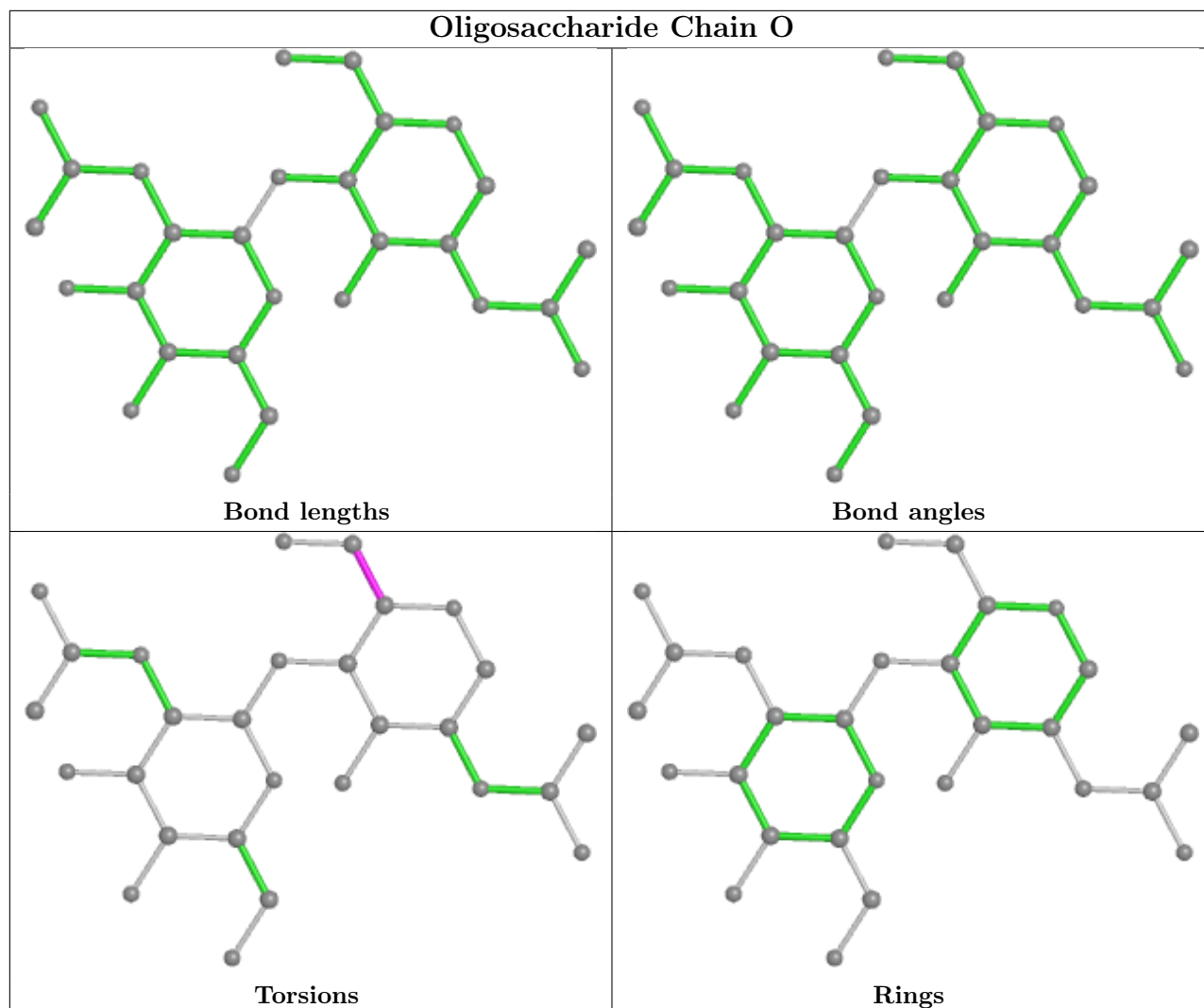












## 5.6 Ligand geometry [i](#)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	C	1303	1	14,14,15	0.18	0	17,19,21	0.58	0
3	NAG	A	1305	1	14,14,15	0.32	0	17,19,21	0.51	0
3	NAG	C	1307	1	14,14,15	0.40	0	17,19,21	0.54	0
3	NAG	B	1315	1	14,14,15	0.19	0	17,19,21	0.61	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1309	1	14,14,15	0.23	0	17,19,21	0.58	0
3	NAG	A	1301	1	14,14,15	0.40	0	17,19,21	0.54	0
3	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.52	0
3	NAG	C	1304	1	14,14,15	0.50	0	17,19,21	0.71	0
3	NAG	B	1309	1	14,14,15	0.22	0	17,19,21	0.58	0
3	NAG	A	1309	1	14,14,15	0.22	0	17,19,21	0.58	0
3	NAG	A	1302	1	14,14,15	0.41	0	17,19,21	0.87	1 (5%)
3	NAG	B	1307	1	14,14,15	0.40	0	17,19,21	0.55	0
3	NAG	C	1301	1	14,14,15	0.40	0	17,19,21	0.54	0
3	NAG	A	1320	1	14,14,15	0.45	0	17,19,21	0.57	0
3	NAG	B	1303	1	14,14,15	0.18	0	17,19,21	0.59	0
3	NAG	B	1320	1	14,14,15	0.44	0	17,19,21	0.57	0
3	NAG	C	1302	1	14,14,15	0.41	0	17,19,21	0.87	1 (5%)
3	NAG	C	1305	1	14,14,15	0.32	0	17,19,21	0.52	0
3	NAG	A	1315	1	14,14,15	0.20	0	17,19,21	0.61	0
3	NAG	C	1306	1	14,14,15	0.15	0	17,19,21	0.61	0
3	NAG	C	1310	1	14,14,15	0.25	0	17,19,21	0.57	0
3	NAG	B	1301	1	14,14,15	0.39	0	17,19,21	0.54	0
3	NAG	C	1308	1	14,14,15	0.39	0	17,19,21	1.46	2 (11%)
3	NAG	A	1306	1	14,14,15	0.16	0	17,19,21	0.62	0
3	NAG	A	1303	1	14,14,15	0.19	0	17,19,21	0.58	0
3	NAG	A	1310	1	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	C	1315	1	14,14,15	0.20	0	17,19,21	0.61	0
3	NAG	B	1306	1	14,14,15	0.16	0	17,19,21	0.61	0
3	NAG	C	1320	1	14,14,15	0.43	0	17,19,21	0.57	0
3	NAG	A	1307	1	14,14,15	0.39	0	17,19,21	0.55	0
3	NAG	B	1304	1	14,14,15	0.50	0	17,19,21	0.72	0
3	NAG	B	1308	1	14,14,15	0.38	0	17,19,21	1.46	2 (11%)
3	NAG	A	1304	1	14,14,15	0.51	0	17,19,21	0.71	0
3	NAG	B	1302	1	14,14,15	0.39	0	17,19,21	0.88	1 (5%)
3	NAG	B	1310	1	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	A	1308	1	14,14,15	0.38	0	17,19,21	1.45	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
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1315	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1320	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1320	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1315	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	5/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1315	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1320	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	5/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1308	NAG	C2-N2-C7	4.53	129.36	122.90
3	B	1308	NAG	C2-N2-C7	4.49	129.30	122.90
3	A	1308	NAG	C2-N2-C7	4.46	129.25	122.90
3	B	1302	NAG	C2-N2-C7	2.77	126.85	122.90
3	A	1302	NAG	C2-N2-C7	2.77	126.85	122.90
3	C	1302	NAG	C2-N2-C7	2.75	126.81	122.90
3	A	1308	NAG	C1-C2-N2	2.52	114.80	110.49
3	B	1308	NAG	C1-C2-N2	2.50	114.77	110.49
3	C	1308	NAG	C1-C2-N2	2.49	114.74	110.49

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1306	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	C	1306	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	A	1315	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	B	1315	NAG	O5-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	C	1315	NAG	O5-C5-C6-O6
3	A	1306	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	A	1315	NAG	C4-C5-C6-O6
3	A	1302	NAG	C8-C7-N2-C2
3	A	1302	NAG	O7-C7-N2-C2
3	A	1308	NAG	C8-C7-N2-C2
3	A	1308	NAG	O7-C7-N2-C2
3	B	1302	NAG	C8-C7-N2-C2
3	B	1302	NAG	O7-C7-N2-C2
3	B	1308	NAG	C8-C7-N2-C2
3	B	1308	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	C	1308	NAG	C8-C7-N2-C2
3	C	1308	NAG	O7-C7-N2-C2
3	A	1302	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	B	1315	NAG	C4-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	C	1315	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	B	1303	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	A	1320	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	B	1320	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	C	1320	NAG	O5-C5-C6-O6
3	A	1309	NAG	O5-C5-C6-O6
3	B	1309	NAG	O5-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	A	1310	NAG	O5-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	A	1308	NAG	C3-C2-N2-C7
3	B	1308	NAG	C3-C2-N2-C7
3	B	1320	NAG	C3-C2-N2-C7
3	C	1308	NAG	C3-C2-N2-C7
3	C	1320	NAG	C3-C2-N2-C7
3	A	1320	NAG	C1-C2-N2-C7
3	B	1320	NAG	C1-C2-N2-C7
3	C	1320	NAG	C1-C2-N2-C7
3	A	1304	NAG	C1-C2-N2-C7
3	B	1304	NAG	C1-C2-N2-C7
3	C	1304	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	A	1320	NAG	C3-C2-N2-C7
3	B	1308	NAG	C1-C2-N2-C7
3	A	1308	NAG	C1-C2-N2-C7
3	C	1308	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1304	NAG	1	0
3	C	1308	NAG	1	0
3	B	1304	NAG	2	0
3	B	1308	NAG	1	0
3	A	1304	NAG	2	0
3	A	1308	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.

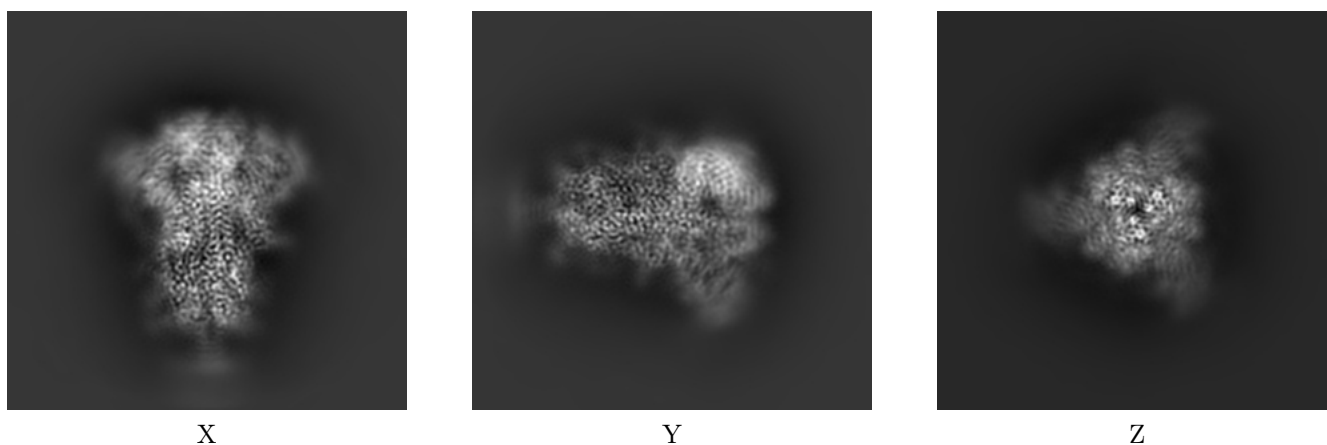
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11332. 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](#)

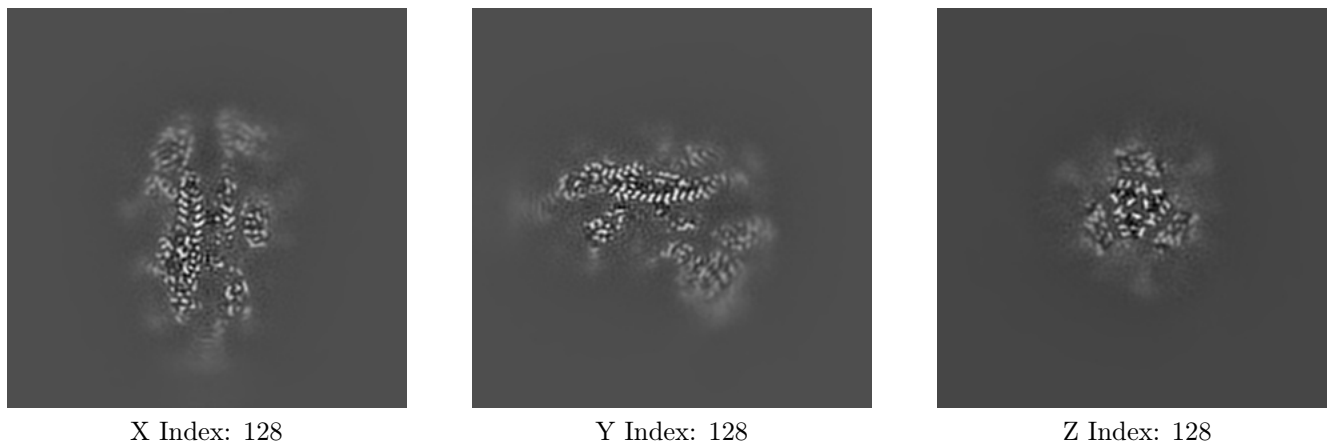
#### 6.1.1 Primary map



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

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

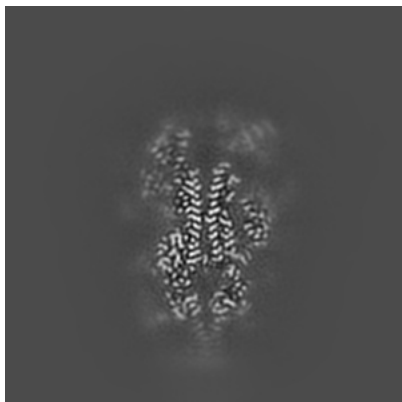
#### 6.2.1 Primary map



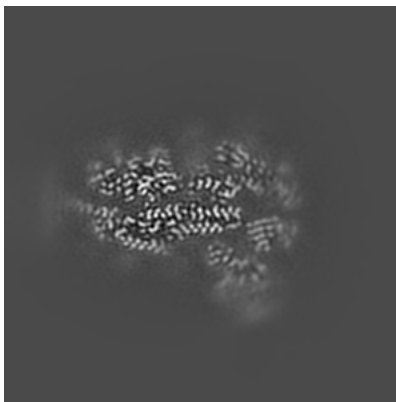
The images above show central slices of the map in three orthogonal directions.

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

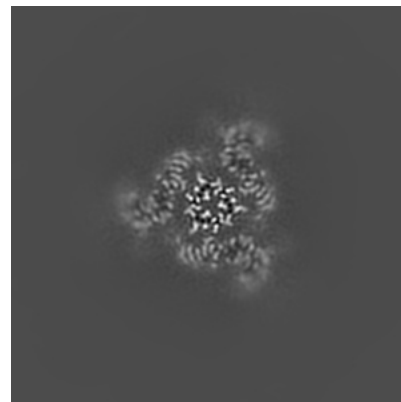
### 6.3.1 Primary map



X Index: 125



Y Index: 135



Z Index: 139

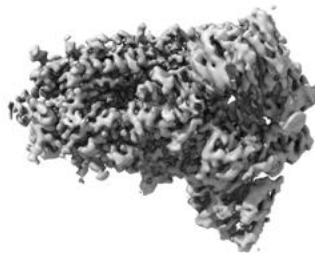
The images above show the largest variance slices of the map in three orthogonal directions.

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

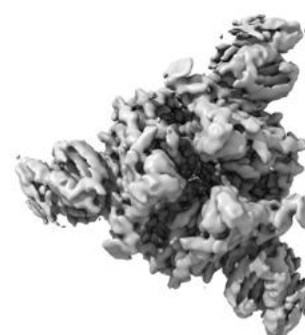
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0222. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

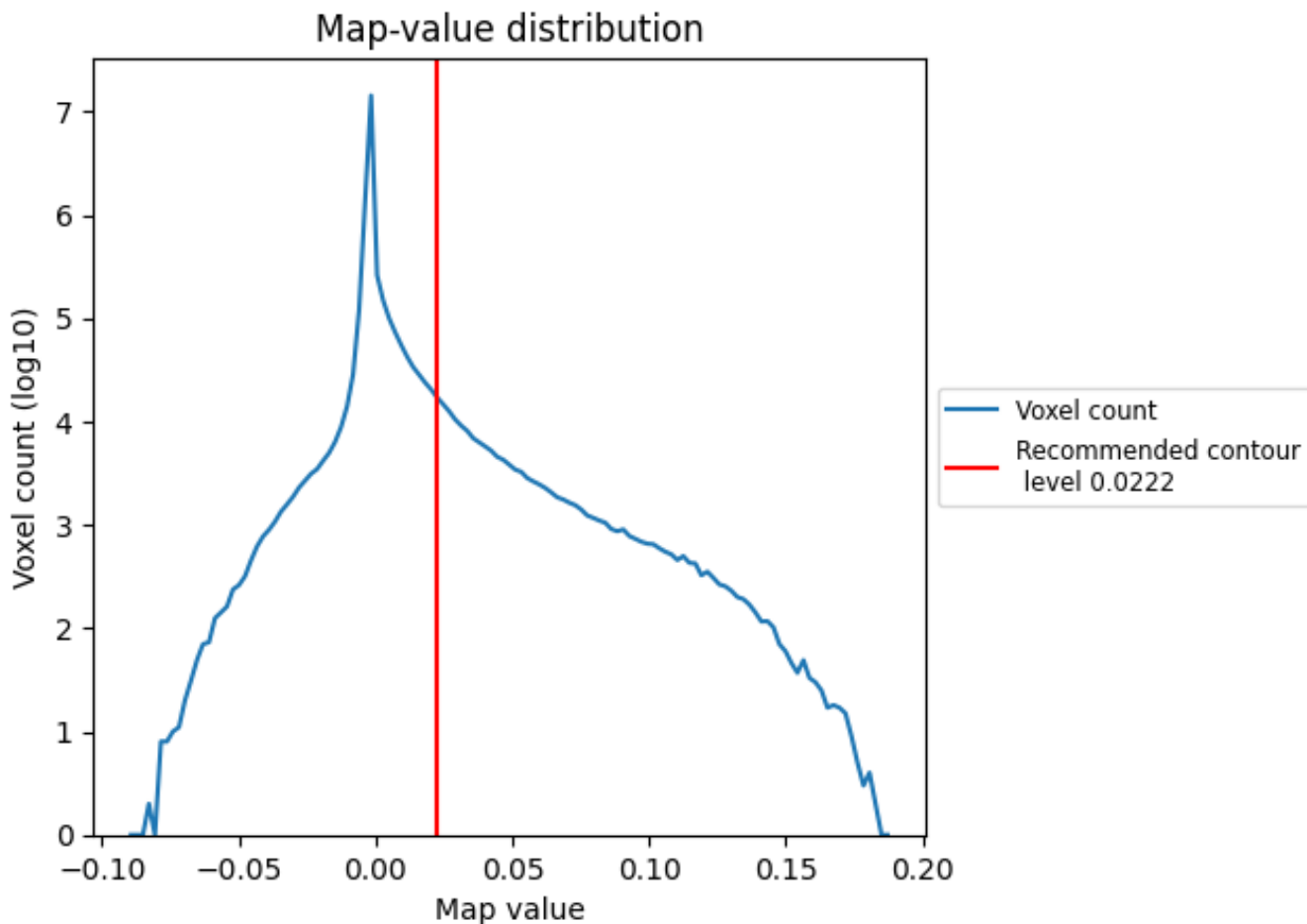
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

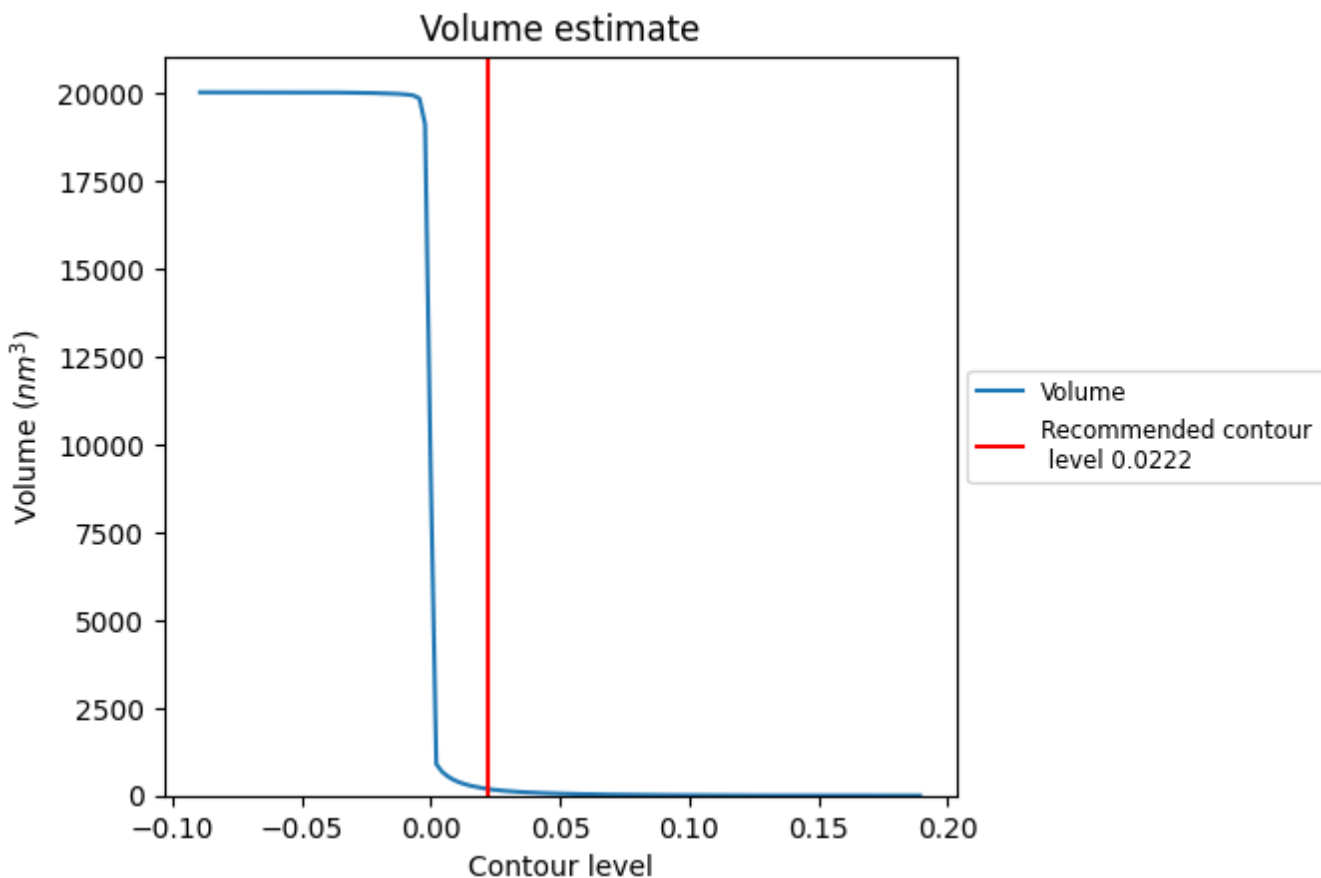
This section contains the results of statistical analysis of the map.

### 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.

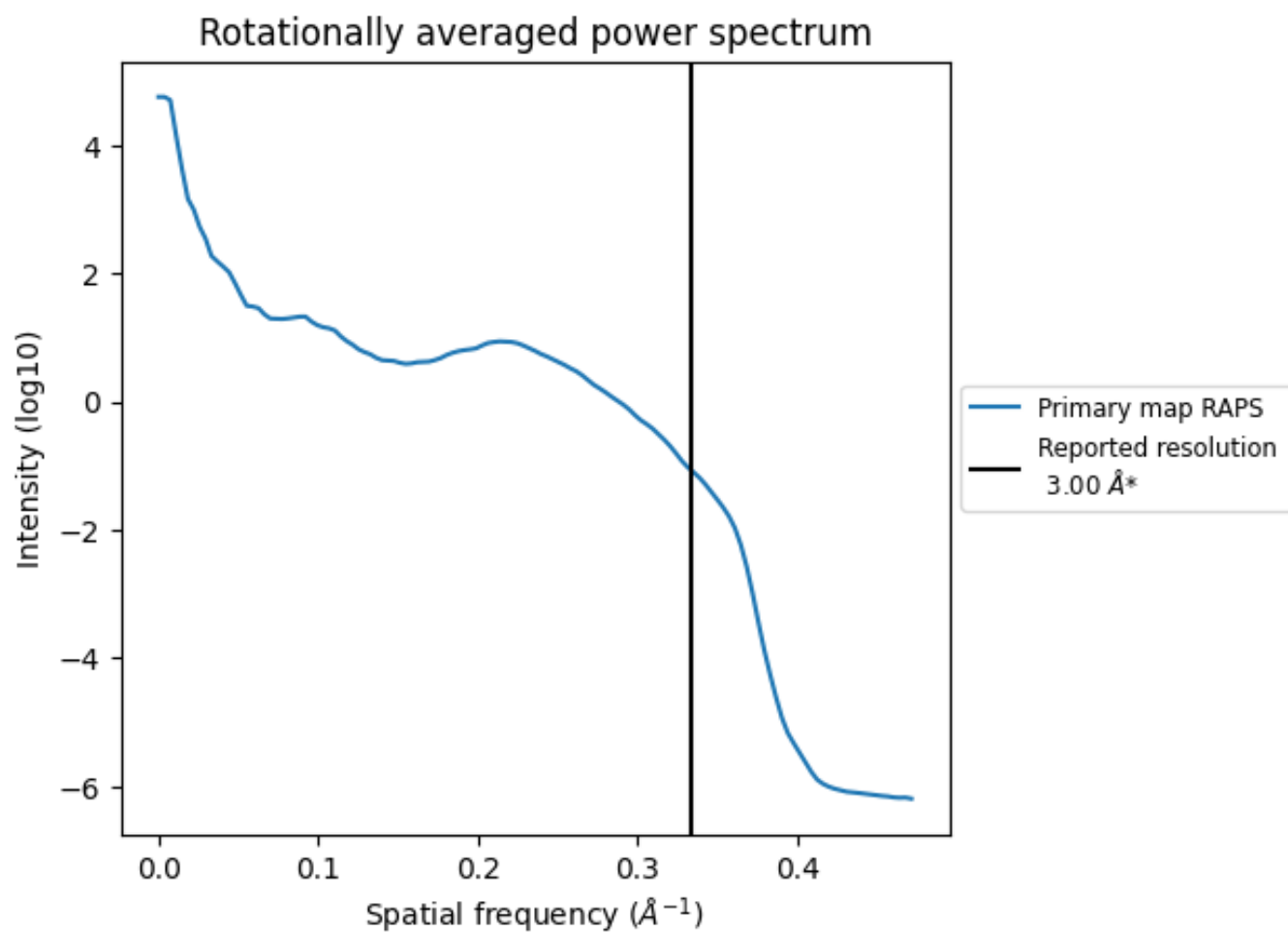
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 187  $\text{nm}^3$ ; this corresponds to an approximate mass of 169 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 i



\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

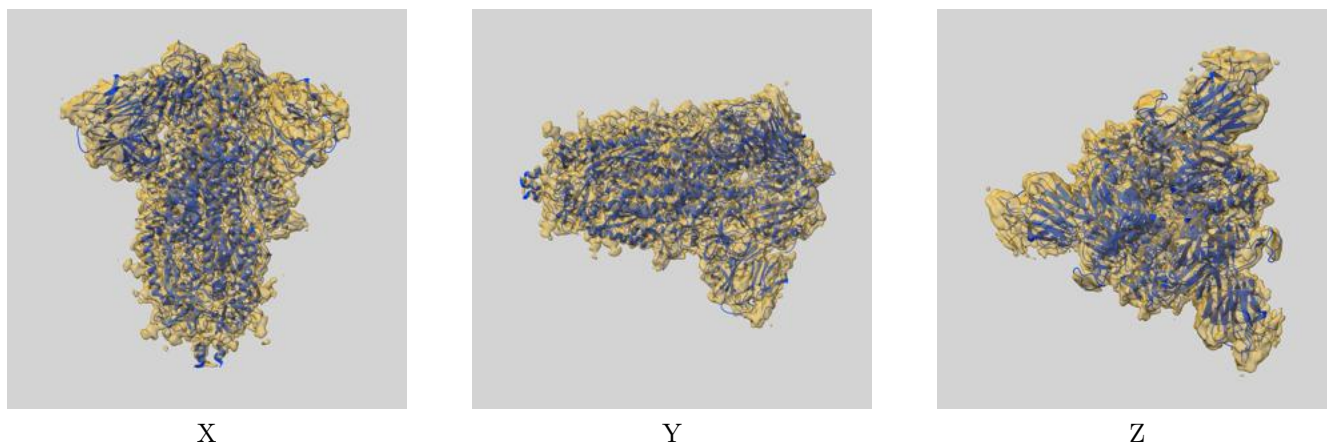
## 8 Fourier-Shell correlation

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

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

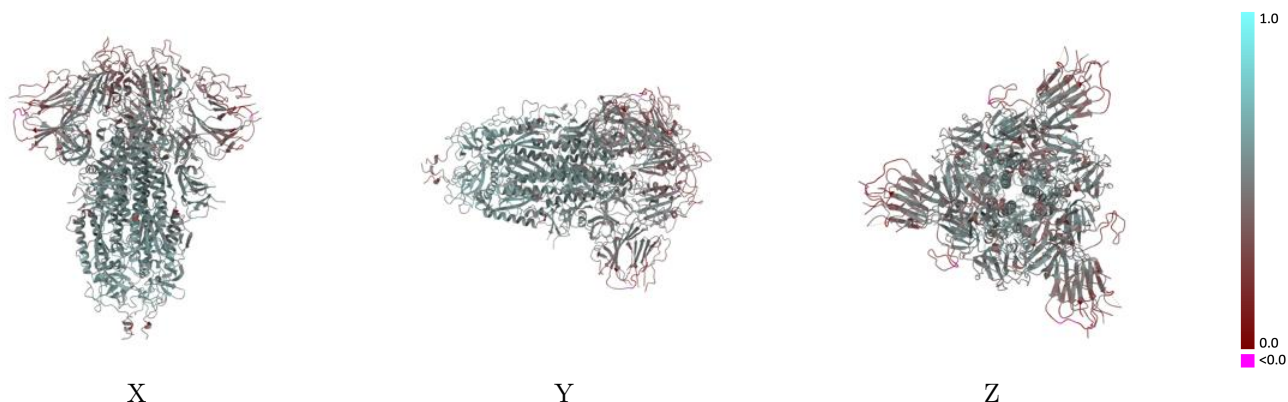
This section contains information regarding the fit between EMDB map EMD-11332 and PDB model 6ZP0. Per-residue inclusion information can be found in section 3 on page 12.

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



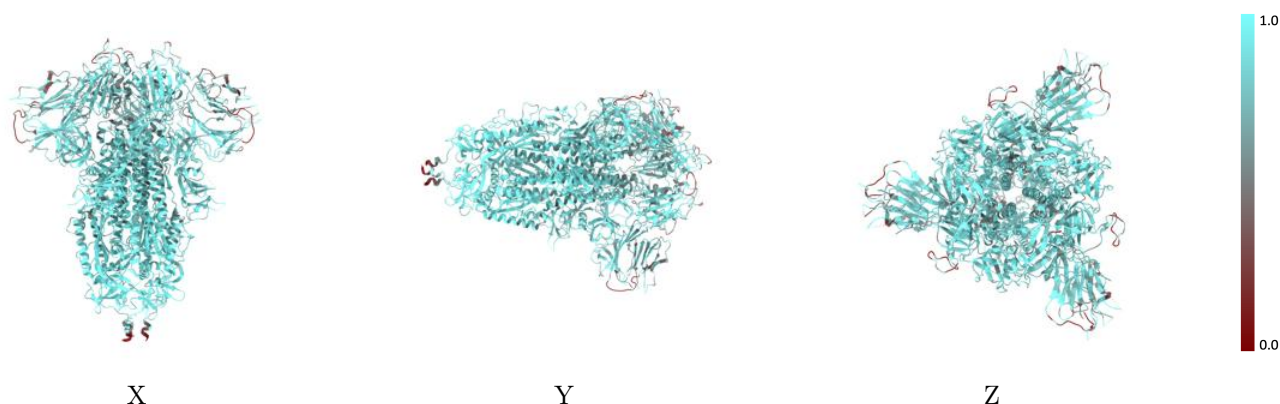
The images above show the 3D surface view of the map at the recommended contour level 0.0222 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



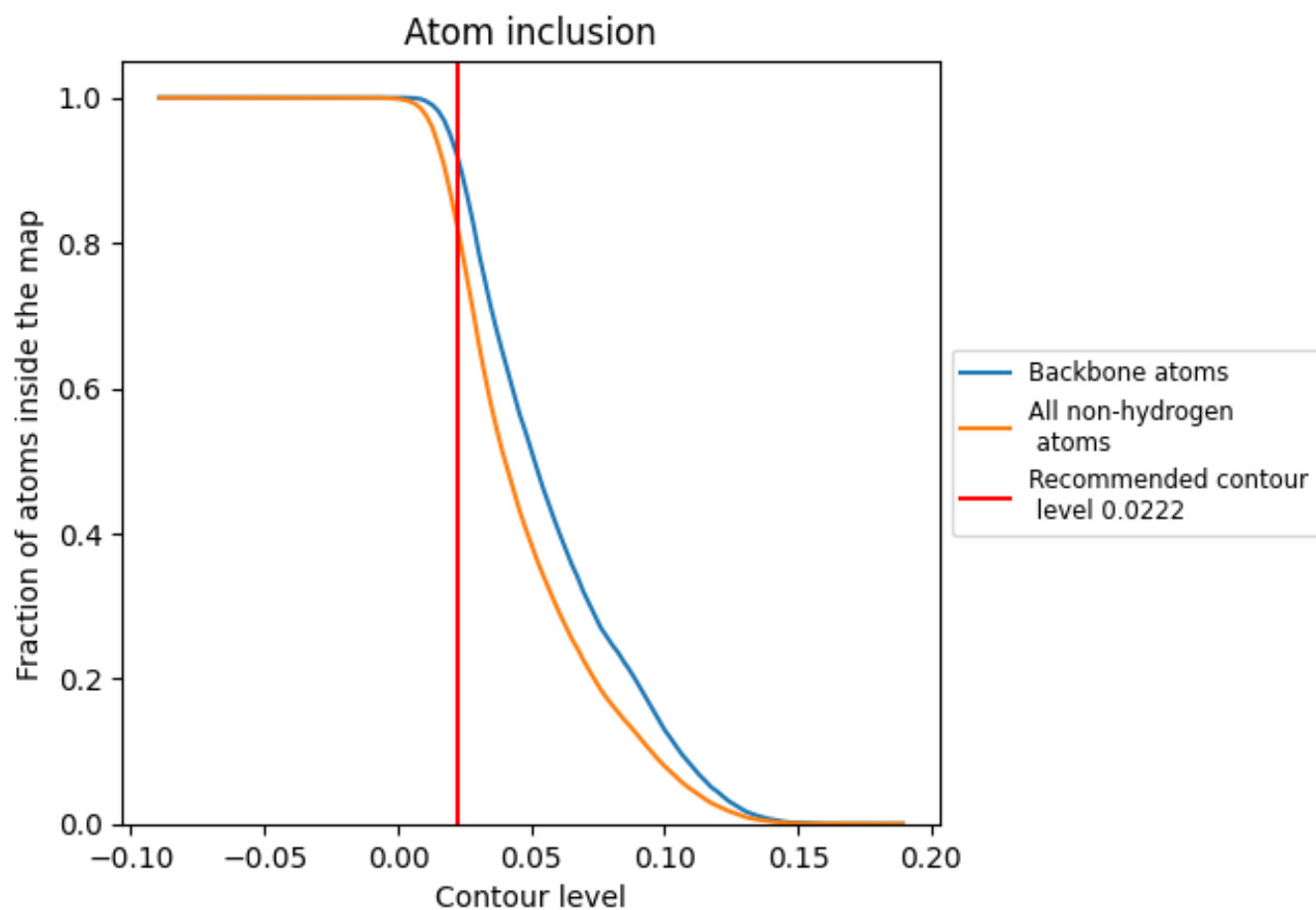
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0222).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.0222) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8256	 0.4830
A	 0.8267	 0.4840
B	 0.8268	 0.4830
C	 0.8254	 0.4840
D	 0.8214	 0.5250
E	 0.7857	 0.4480
F	 0.7857	 0.4690
G	 0.7143	 0.4760
H	 0.8214	 0.5280
I	 0.7857	 0.4570
J	 0.7857	 0.4710
K	 0.6786	 0.4660
L	 0.8214	 0.5310
M	 0.7857	 0.4560
N	 0.7857	 0.4740
O	 0.6786	 0.4920

