



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 05:11 am BST

PDB ID : 6ZOY  
EMDB ID : EMD-11330  
Title : Structure of Disulphide-stabilized SARS-CoV-2 Spike Protein Trimer (x1 disulphide-bond mutant, S383C, D985C, K986P, V987P, 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 : 3.10 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.dev113  
Mogul : 1.8.4, 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

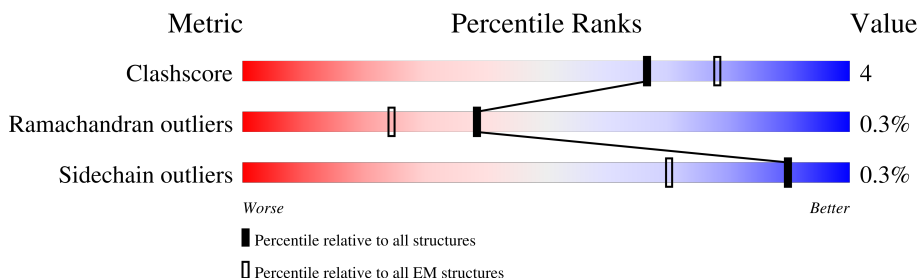
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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	1247	73% 8% 18%
1	B	1247	74% 8% 18%
1	C	1247	74% 8% 18%
2	D	2	100%
2	E	2	100%
2	F	2	50% 100%
2	G	2	100%
2	H	2	100%

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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

There are 3 unique types of molecules in this entry. The entry contains 24753 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1021	Total	C	N	O	S	0	0
			7971	5088	1326	1518	39		
1	B	1021	Total	C	N	O	S	0	0
			7971	5088	1326	1518	39		
1	C	1021	Total	C	N	O	S	0	0
			7971	5088	1326	1518	39		

There are 183 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	383	CYS	SER	engineered mutation	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	985	CYS	ASP	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLY	-	expression tag	UNP P0DTC2
A	1226	SER	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	TYR	-	expression tag	UNP P0DTC2
A	1229	ILE	-	expression tag	UNP P0DTC2
A	1230	PRO	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	ALA	-	expression tag	UNP P0DTC2
A	1233	PRO	-	expression tag	UNP P0DTC2
A	1234	ARG	-	expression tag	UNP P0DTC2
A	1235	ASP	-	expression tag	UNP P0DTC2
A	1236	GLY	-	expression tag	UNP P0DTC2
A	1237	GLN	-	expression tag	UNP P0DTC2
A	1238	ALA	-	expression tag	UNP P0DTC2
A	1239	TYR	-	expression tag	UNP P0DTC2
A	1240	VAL	-	expression tag	UNP P0DTC2
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	383	CYS	SER	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	985	CYS	ASP	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1212	GLY	-	expression tag	UNP P0DTC2
B	1213	SER	-	expression tag	UNP P0DTC2
B	1214	GLY	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	GLU	-	expression tag	UNP P0DTC2
B	1217	ASN	-	expression tag	UNP P0DTC2
B	1218	LEU	-	expression tag	UNP P0DTC2
B	1219	TYR	-	expression tag	UNP P0DTC2
B	1220	PHE	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLY	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	SER	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	TYR	-	expression tag	UNP P0DTC2
B	1229	ILE	-	expression tag	UNP P0DTC2
B	1230	PRO	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	ALA	-	expression tag	UNP P0DTC2
B	1233	PRO	-	expression tag	UNP P0DTC2
B	1234	ARG	-	expression tag	UNP P0DTC2
B	1235	ASP	-	expression tag	UNP P0DTC2
B	1236	GLY	-	expression tag	UNP P0DTC2
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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1247	VAL	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	LEU	-	expression tag	UNP P0DTC2
B	1250	SER	-	expression tag	UNP P0DTC2
B	1251	THR	-	expression tag	UNP P0DTC2
B	1252	PHE	-	expression tag	UNP P0DTC2
B	1253	LEU	-	expression tag	UNP P0DTC2
B	1254	GLY	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
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	383	CYS	SER	engineered mutation	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	985	CYS	ASP	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

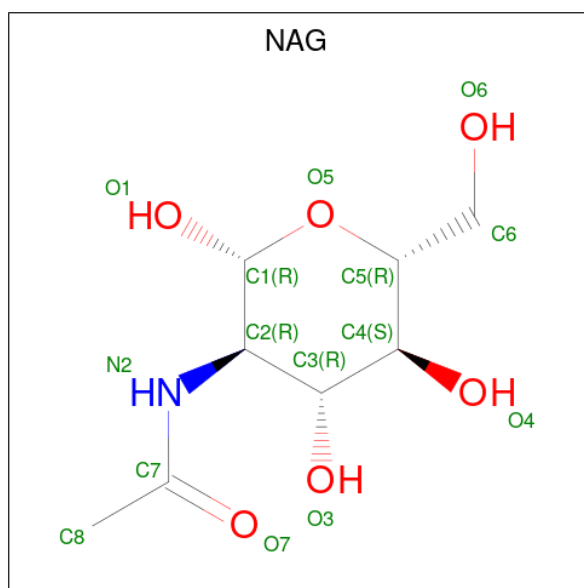
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





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

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



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

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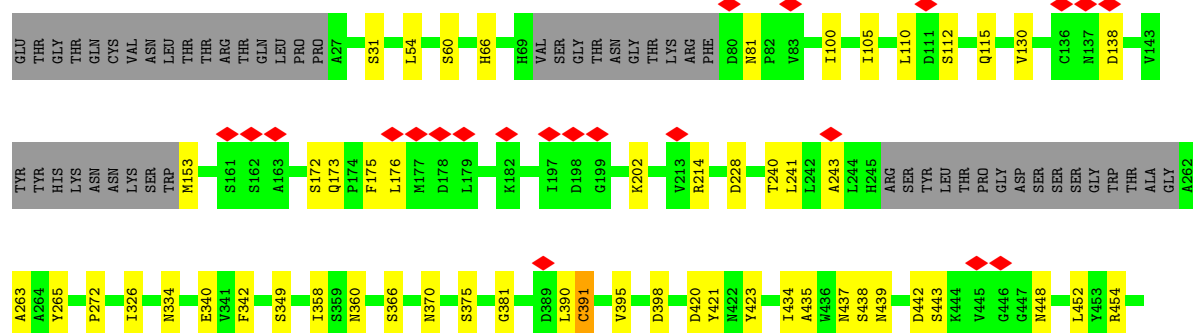
Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3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

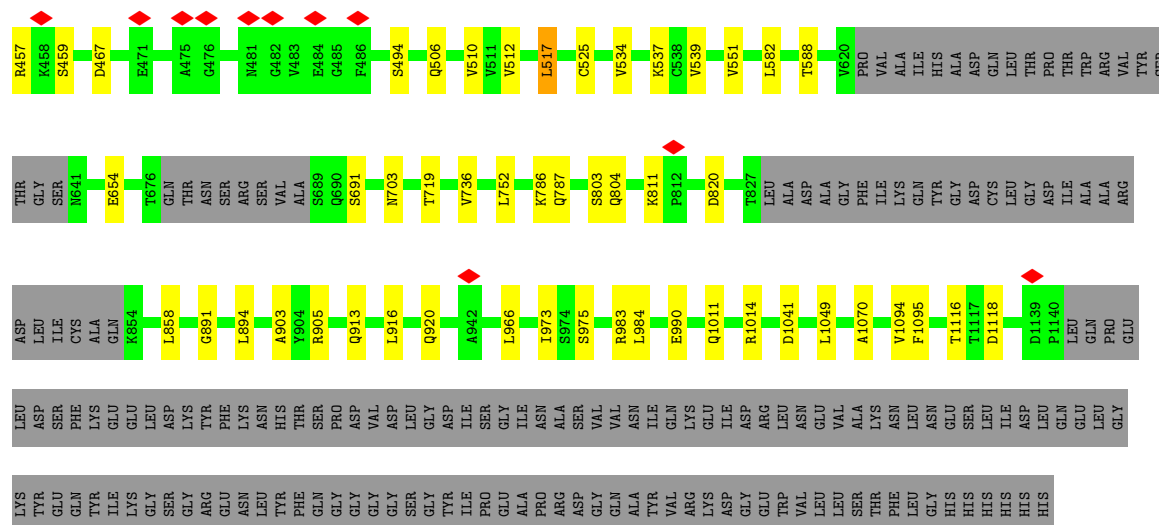


Frequency	Percentage
Daily	74%
Weekly	8%
Monthly	18%



Category	Percentage
Very bad	74%
Bad	8%
Good	18%





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

Chain D:  100%

NAG1  
NAG2

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

Chain E:  100%

NAG1  
NAG2

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

Chain F:  50%  100%

NAG1  
NAG2

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

Chain G:  100%

NAG1  
NAG2

- 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%

WAG1  
WAG2

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

Chain K:  100%

WAG1  
WAG2

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

Chain L:  100%

WAG1  
WAG2

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

Chain M:  100%

WAG1  
WAG2

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

Chain N:  100%

WAG1  
WAG2

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

Chain O:  100%

MOL  
MOL2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	210946	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	0.192	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0211	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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.49	0/8151	0.71	2/11088 (0.0%)
1	B	0.49	0/8151	0.71	2/11088 (0.0%)
1	C	0.49	0/8151	0.71	2/11088 (0.0%)
All	All	0.49	0/24453	0.71	6/33264 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	391	CYS	CA-CB-SG	7.69	127.84	114.00
1	A	391	CYS	CA-CB-SG	7.68	127.82	114.00
1	B	391	CYS	CA-CB-SG	7.67	127.81	114.00
1	C	517	LEU	CA-CB-CG	6.40	130.03	115.30
1	B	517	LEU	CA-CB-CG	6.40	130.03	115.30
1	A	517	LEU	CA-CB-CG	6.39	130.00	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	7971	0	7762	64	0
1	B	7971	0	7762	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7971	0	7762	63	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	1	0
3	B	168	0	156	1	0
3	C	168	0	156	1	0
All	All	24753	0	24054	181	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 4.

All (181) 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:811:LYS:NZ	1:B:820:ASP:OD2	2.14	0.80
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.14	0.80
1:A:703:ASN:ND2	1:B:787:GLN:OE1	2.15	0.79
1:A:787:GLN:OE1	1:C:703:ASN:ND2	2.14	0.79
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.14	0.79
1:B:703:ASN:ND2	1:C:787:GLN:OE1	2.16	0.78
1:B:1116:THR:OG1	1:B:1118:ASP:OD1	2.04	0.76
1:C:1116:THR:OG1	1:C:1118:ASP:OD1	2.04	0.76
1:A:1116:THR:OG1	1:A:1118:ASP:OD1	2.04	0.75
1:A:439:ASN:ND2	1:A:506:GLN:OE1	2.21	0.73
1:B:439:ASN:ND2	1:B:506:GLN:OE1	2.21	0.73
1:C:439:ASN:ND2	1:C:506:GLN:OE1	2.21	0.73
1:B:654:GLU:OE1	1:B:691:SER:OG	2.09	0.71
1:A:654:GLU:OE1	1:A:691:SER:OG	2.09	0.70
1:C:654:GLU:OE1	1:C:691:SER:OG	2.09	0.69
1:A:803:SER:OG	1:A:804:GLN:OE1	2.12	0.68
1:C:803:SER:OG	1:C:804:GLN:OE1	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:803:SER:OG	1:B:804:GLN:OE1	2.12	0.67
1:A:100:ILE:HA	1:A:243:ALA:HB3	1.78	0.65
1:C:100:ILE:HA	1:C:243:ALA:HB3	1.78	0.64
1:C:66:HIS:ND1	1:C:263:ALA:O	2.31	0.64
1:B:100:ILE:HA	1:B:243:ALA:HB3	1.78	0.63
1:A:66:HIS:ND1	1:A:263:ALA:O	2.31	0.63
1:B:66:HIS:ND1	1:B:263:ALA:O	2.31	0.63
1:B:457:ARG:NE	1:B:467:ASP:OD2	2.32	0.62
1:C:457:ARG:NE	1:C:467:ASP:OD2	2.32	0.62
1:C:1011:GLN:OE1	1:C:1014:ARG:NH1	2.32	0.62
1:A:1011:GLN:OE1	1:A:1014:ARG:NH1	2.32	0.62
1:B:1011:GLN:OE1	1:B:1014:ARG:NH1	2.32	0.62
1:C:752:LEU:HD11	1:C:990:GLU:OE1	2.00	0.61
1:B:334:ASN:ND2	1:B:360:ASN:O	2.34	0.61
1:C:334:ASN:ND2	1:C:360:ASN:O	2.34	0.61
1:A:752:LEU:HD11	1:A:990:GLU:OE1	2.01	0.60
1:B:752:LEU:HD11	1:B:990:GLU:OE1	2.00	0.60
1:A:736:VAL:HG22	1:A:858:LEU:HD13	1.84	0.60
1:A:334:ASN:ND2	1:A:360:ASN:O	2.34	0.59
1:B:736:VAL:HG22	1:B:858:LEU:HD13	1.84	0.59
1:C:736:VAL:HG22	1:C:858:LEU:HD13	1.84	0.59
1:A:81:ASN:ND2	1:A:265:TYR:OH	2.36	0.58
1:B:81:ASN:ND2	1:B:265:TYR:OH	2.36	0.58
1:A:457:ARG:NE	1:A:467:ASP:OD2	2.32	0.58
1:C:81:ASN:ND2	1:C:265:TYR:OH	2.36	0.57
1:A:349:SER:OG	1:A:452:LEU:O	2.23	0.57
1:B:786:LYS:NZ	1:B:891:GLY:O	2.39	0.56
1:B:349:SER:OG	1:B:452:LEU:O	2.23	0.56
1:A:786:LYS:NZ	1:A:891:GLY:O	2.39	0.56
1:C:457:ARG:NH1	1:C:459:SER:OG	2.39	0.56
1:A:457:ARG:NH1	1:A:459:SER:OG	2.39	0.56
1:B:439:ASN:O	1:B:443:SER:OG	2.24	0.55
1:B:457:ARG:NH1	1:B:459:SER:OG	2.39	0.55
1:C:349:SER:OG	1:C:452:LEU:O	2.23	0.55
1:C:439:ASN:O	1:C:443:SER:OG	2.24	0.55
1:C:31:SER:HG	1:C:60:SER:N	2.05	0.55
1:B:366:SER:O	1:B:370:ASN:ND2	2.40	0.55
1:C:786:LYS:NZ	1:C:891:GLY:O	2.39	0.55
1:C:366:SER:O	1:C:370:ASN:ND2	2.40	0.55
1:A:439:ASN:O	1:A:443:SER:OG	2.24	0.54
1:A:342:PHE:HE1	1:A:434:ILE:HG21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:SER:O	1:A:370:ASN:ND2	2.40	0.54
1:B:31:SER:HG	1:B:60:SER:N	2.06	0.54
1:C:342:PHE:HE1	1:C:434:ILE:HG21	1.73	0.54
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.40	0.53
1:A:31:SER:HG	1:A:60:SER:N	2.06	0.53
1:B:340:GLU:N	1:B:340:GLU:OE1	2.42	0.53
1:B:435:ALA:HB2	1:B:510:VAL:HG12	1.91	0.52
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.40	0.52
1:C:435:ALA:HB2	1:C:510:VAL:HG12	1.92	0.52
1:C:966:LEU:O	1:C:975:SER:OG	2.28	0.52
1:B:342:PHE:HE1	1:B:434:ILE:HG21	1.73	0.52
1:B:966:LEU:O	1:B:975:SER:OG	2.28	0.52
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.40	0.51
1:A:435:ALA:HB2	1:A:510:VAL:HG12	1.91	0.51
1:C:442:ASP:O	1:C:448:ASN:ND2	2.42	0.51
1:A:340:GLU:N	1:A:340:GLU:OE1	2.42	0.49
1:A:966:LEU:O	1:A:975:SER:OG	2.28	0.49
1:B:381:GLY:O	1:C:984:LEU:HD21	2.12	0.49
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.95	0.49
1:B:358:ILE:HB	1:B:395:VAL:HG13	1.95	0.48
1:C:202:LYS:NZ	1:C:228:ASP:OD2	2.43	0.48
1:C:358:ILE:HB	1:C:395:VAL:HG13	1.95	0.48
1:A:442:ASP:O	1:A:448:ASN:ND2	2.42	0.48
1:B:442:ASP:O	1:B:448:ASN:ND2	2.42	0.48
1:C:340:GLU:OE1	1:C:340:GLU:N	2.42	0.48
1:A:983:ARG:NH1	1:C:381:GLY:O	2.47	0.47
1:B:391:CYS:HB2	1:B:525:CYS:HA	1.96	0.47
1:B:437:ASN:OD1	1:B:438:SER:N	2.47	0.47
1:C:391:CYS:HB2	1:C:525:CYS:HA	1.96	0.47
1:A:391:CYS:HB2	1:A:525:CYS:HA	1.96	0.47
1:C:105:ILE:CG2	1:C:110:LEU:HD23	2.45	0.47
1:B:105:ILE:CG2	1:B:110:LEU:HD23	2.45	0.47
1:C:437:ASN:OD1	1:C:438:SER:N	2.47	0.47
1:B:202:LYS:NZ	1:B:228:ASP:OD2	2.43	0.47
1:A:105:ILE:CG2	1:A:110:LEU:HD23	2.45	0.47
1:A:437:ASN:OD1	1:A:438:SER:N	2.47	0.47
1:B:326:ILE:HD12	1:B:539:VAL:HG21	1.96	0.47
1:B:452:LEU:HD23	1:B:494:SER:HB2	1.96	0.47
1:C:326:ILE:HD12	1:C:539:VAL:HG21	1.96	0.47
1:B:390:LEU:HD11	1:C:983:ARG:CB	2.44	0.46
1:B:375:SER:N	1:B:435:ALA:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:LEU:HD23	1:C:494:SER:HB2	1.97	0.46
1:A:375:SER:N	1:A:435:ALA:O	2.48	0.46
1:A:390:LEU:HD11	1:B:983:ARG:CB	2.45	0.46
1:B:551:VAL:HG12	1:B:588:THR:O	2.16	0.46
1:C:175:PHE:O	1:C:176:LEU:HD22	2.16	0.46
1:C:551:VAL:HG12	1:C:588:THR:O	2.16	0.46
1:A:326:ILE:HD12	1:A:539:VAL:HG21	1.96	0.46
1:B:719:THR:HG23	1:B:1070:ALA:HB2	1.98	0.46
1:A:381:GLY:O	1:B:983:ARG:NH1	2.49	0.46
1:A:452:LEU:HD23	1:A:494:SER:HB2	1.97	0.46
1:A:719:THR:HG23	1:A:1070:ALA:HB2	1.98	0.45
1:A:175:PHE:O	1:A:176:LEU:HD22	2.16	0.45
1:B:175:PHE:O	1:B:176:LEU:HD22	2.16	0.45
1:B:537:LYS:N	1:B:551:VAL:HG23	2.32	0.45
1:A:537:LYS:N	1:A:551:VAL:HG23	2.32	0.45
1:A:551:VAL:HG12	1:A:588:THR:O	2.16	0.45
1:C:537:LYS:N	1:C:551:VAL:HG23	2.32	0.45
1:C:719:THR:HG23	1:C:1070:ALA:HB2	1.98	0.45
1:A:31:SER:OG	1:A:60:SER:N	2.50	0.45
1:C:375:SER:N	1:C:435:ALA:O	2.48	0.45
1:B:391:CYS:CB	1:B:525:CYS:HA	2.47	0.45
1:C:391:CYS:CB	1:C:525:CYS:HA	2.47	0.45
1:A:202:LYS:NZ	1:A:228:ASP:OD2	2.43	0.45
1:B:31:SER:OG	1:B:60:SER:N	2.50	0.45
3:A:1308:NAG:H83	3:A:1308:NAG:H3	1.99	0.44
1:C:916:LEU:O	1:C:920:GLN:N	2.51	0.44
1:B:54:LEU:HD23	1:B:272:PRO:HA	1.99	0.44
1:A:391:CYS:CB	1:A:525:CYS:HA	2.47	0.44
1:A:153:MET:SD	1:A:153:MET:N	2.91	0.44
3:B:1308:NAG:H83	3:B:1308:NAG:H3	2.00	0.44
1:C:153:MET:N	1:C:153:MET:SD	2.91	0.44
1:C:31:SER:OG	1:C:60:SER:N	2.50	0.43
1:B:153:MET:SD	1:B:153:MET:N	2.91	0.43
1:C:54:LEU:HD23	1:C:272:PRO:HA	1.99	0.43
1:A:54:LEU:HD23	1:A:272:PRO:HA	1.99	0.43
1:B:115:GLN:NE2	1:B:130:VAL:O	2.52	0.43
1:B:916:LEU:O	1:B:920:GLN:N	2.51	0.43
1:A:326:ILE:HD11	1:A:534:VAL:HG12	2.00	0.43
3:C:1308:NAG:H83	3:C:1308:NAG:H3	1.99	0.43
1:A:916:LEU:O	1:A:920:GLN:N	2.51	0.43
1:B:326:ILE:HD11	1:B:534:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:PRO:HD3	1:C:894:LEU:HD13	2.01	0.43
1:A:903:ALA:HB1	1:A:913:GLN:HB2	2.01	0.43
1:A:983:ARG:CB	1:C:390:LEU:HD11	2.49	0.43
1:C:172:SER:OG	1:C:173:GLN:N	2.52	0.43
1:C:326:ILE:HD11	1:C:534:VAL:HG12	2.00	0.43
1:A:172:SER:OG	1:A:173:GLN:N	2.52	0.43
1:C:115:GLN:NE2	1:C:130:VAL:O	2.52	0.43
1:B:420:ASP:OD1	1:B:421:TYR:N	2.53	0.42
1:A:115:GLN:NE2	1:A:130:VAL:O	2.52	0.42
1:A:715:PRO:HD3	1:B:894:LEU:HD13	2.00	0.42
1:C:454:ARG:NH2	1:C:467:ASP:O	2.46	0.42
1:A:420:ASP:OD1	1:A:421:TYR:N	2.52	0.42
1:C:435:ALA:CB	1:C:510:VAL:HG12	2.50	0.42
1:C:903:ALA:HB1	1:C:913:GLN:HB2	2.01	0.42
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.38	0.42
1:C:420:ASP:OD1	1:C:421:TYR:N	2.53	0.42
1:C:240:THR:HG22	1:C:241:LEU:H	1.85	0.42
1:B:398:ASP:HB2	1:B:512:VAL:HG22	2.02	0.42
1:A:105:ILE:HG22	1:A:110:LEU:HD23	2.02	0.41
1:B:398:ASP:OD2	1:B:423:TYR:OH	2.38	0.41
1:A:973:ILE:HD12	1:A:983:ARG:NH2	2.36	0.41
1:B:903:ALA:HB1	1:B:913:GLN:HB2	2.01	0.41
1:A:454:ARG:NH2	1:A:467:ASP:O	2.46	0.41
1:A:240:THR:HG22	1:A:241:LEU:H	1.85	0.41
1:A:435:ALA:CB	1:A:510:VAL:HG12	2.49	0.41
1:B:172:SER:OG	1:B:173:GLN:N	2.52	0.41
1:B:240:THR:HG22	1:B:241:LEU:H	1.85	0.41
1:B:435:ALA:CB	1:B:510:VAL:HG12	2.49	0.41
1:A:808:ASP:O	1:A:810:SER:N	2.49	0.41
1:B:454:ARG:NH2	1:B:467:ASP:O	2.46	0.41
1:B:973:ILE:HD12	1:B:983:ARG:NH2	2.36	0.41
1:A:398:ASP:HB2	1:A:512:VAL:HG22	2.02	0.41
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.38	0.41
1:B:1094:VAL:HG12	1:B:1095:PHE:N	2.36	0.41
1:B:105:ILE:HG22	1:B:110:LEU:HD23	2.02	0.40
1:A:984:LEU:HD21	1:C:381:GLY:O	2.20	0.40
1:C:973:ILE:HD12	1:C:983:ARG:NH2	2.36	0.40
1:A:1094:VAL:HG12	1:A:1095:PHE:N	2.36	0.40
1:C:105:ILE:HG22	1:C:110:LEU:HD23	2.02	0.40
1:C:398:ASP:HB2	1:C:512:VAL:HG22	2.02	0.40
1:C:1094:VAL:HG12	1:C:1095:PHE:N	2.36	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	1007/1247 (81%)	957 (95%)	47 (5%)	3 (0%)	37	68
1	B	1007/1247 (81%)	957 (95%)	47 (5%)	3 (0%)	37	68
1	C	1007/1247 (81%)	958 (95%)	46 (5%)	3 (0%)	37	68
All	All	3021/3741 (81%)	2872 (95%)	140 (5%)	9 (0%)	38	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ARG
1	B	214	ARG
1	C	214	ARG
1	A	112	SER
1	A	138	ASP
1	B	112	SER
1	B	138	ASP
1	C	112	SER
1	C	138	ASP

### 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	891/1081 (82%)	888 (100%)	3 (0%)	91	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	891/1081 (82%)	888 (100%)	3 (0%)	91	95
1	C	891/1081 (82%)	888 (100%)	3 (0%)	91	95
All	All	2673/3243 (82%)	2664 (100%)	9 (0%)	90	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	517	LEU
1	A	582	LEU
1	A	1041	ASP
1	B	517	LEU
1	B	582	LEU
1	B	1041	ASP
1	C	517	LEU
1	C	582	LEU
1	C	1041	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	99	ASN
1	A	134	GLN
1	A	607	GLN
1	A	703	ASN
1	A	824	ASN
1	A	1101	HIS
1	A	1119	ASN
1	B	81	ASN
1	B	134	GLN
1	B	607	GLN
1	B	703	ASN
1	B	824	ASN
1	B	1101	HIS
1	B	1119	ASN
1	C	81	ASN
1	C	134	GLN
1	C	439	ASN
1	C	506	GLN
1	C	607	GLN

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Mol	Chain	Res	Type
1	C	703	ASN
1	C	824	ASN
1	C	1101	HIS
1	C	1119	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

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	0.24	0	17,19,21	0.61	0
2	NAG	D	2	2	14,14,15	0.17	0	17,19,21	0.59	0
2	NAG	E	1	1,2	14,14,15	0.37	0	17,19,21	0.66	0
2	NAG	E	2	2	14,14,15	0.18	0	17,19,21	0.61	0
2	NAG	F	1	1,2	14,14,15	0.23	0	17,19,21	0.53	0
2	NAG	F	2	2	14,14,15	0.24	0	17,19,21	0.58	0
2	NAG	G	1	1,2	14,14,15	0.54	0	17,19,21	0.60	0
2	NAG	G	2	2	14,14,15	0.25	0	17,19,21	0.58	0
2	NAG	H	1	1,2	14,14,15	0.23	0	17,19,21	0.62	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	0.37	0	17,19,21	0.66	0
2	NAG	I	2	2	14,14,15	0.20	0	17,19,21	0.60	0
2	NAG	J	1	1,2	14,14,15	0.22	0	17,19,21	0.53	0
2	NAG	J	2	2	14,14,15	0.22	0	17,19,21	0.58	0
2	NAG	K	1	1,2	14,14,15	0.53	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	K	2	2	14,14,15	0.24	0	17,19,21	0.58	0
2	NAG	L	1	1,2	14,14,15	0.24	0	17,19,21	0.62	0
2	NAG	L	2	2	14,14,15	0.17	0	17,19,21	0.60	0
2	NAG	M	1	1,2	14,14,15	0.38	0	17,19,21	0.66	0
2	NAG	M	2	2	14,14,15	0.19	0	17,19,21	0.60	0
2	NAG	N	1	1,2	14,14,15	0.23	0	17,19,21	0.53	0
2	NAG	N	2	2	14,14,15	0.23	0	17,19,21	0.58	0
2	NAG	O	1	1,2	14,14,15	0.54	0	17,19,21	0.60	0
2	NAG	O	2	2	14,14,15	0.24	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	-	2/6/23/26	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	-	2/6/23/26	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	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

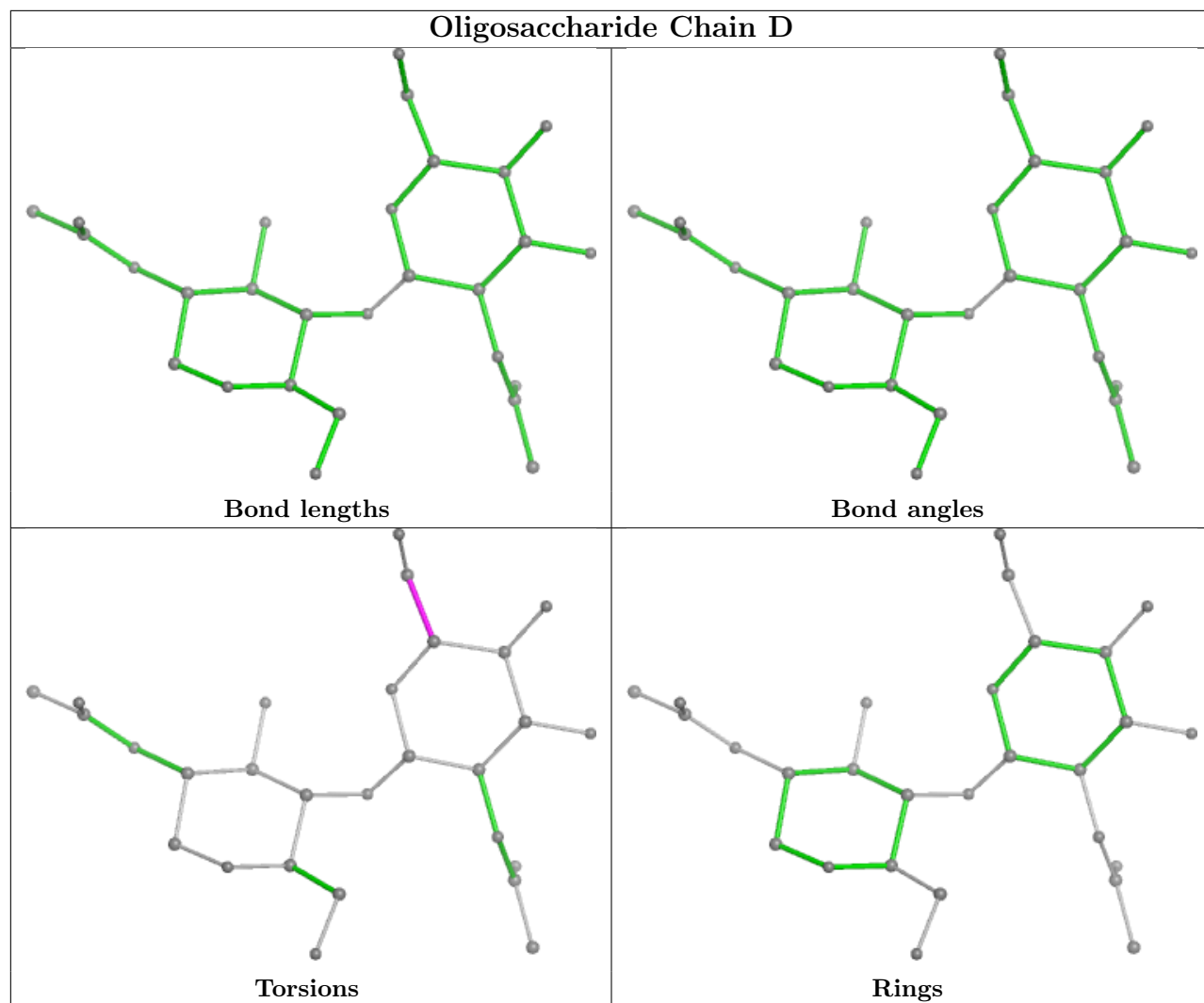
All (27) torsion outliers are listed below:

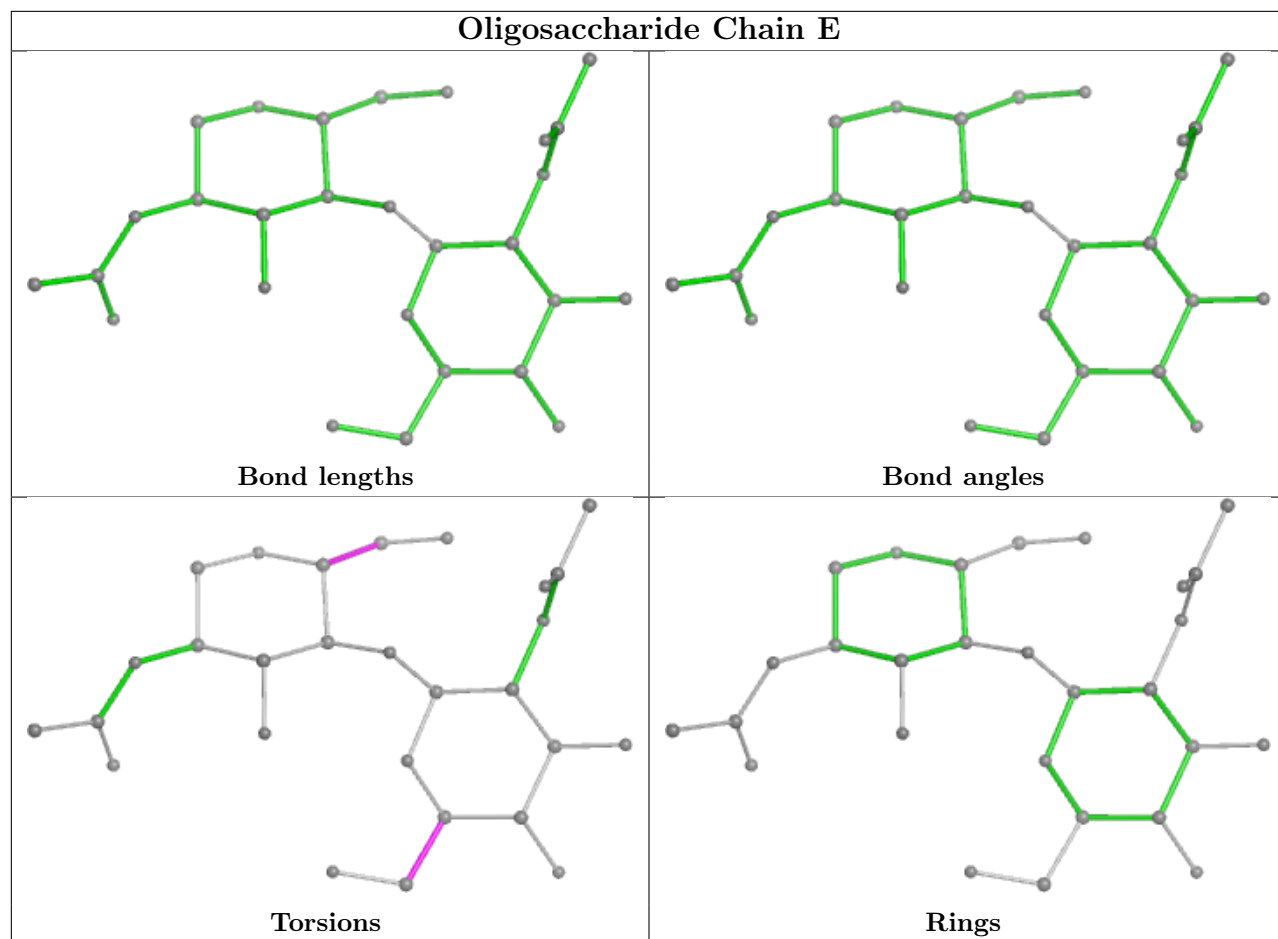
Mol	Chain	Res	Type	Atoms
2	G	1	NAG	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	O	1	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
2	O	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	L	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6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

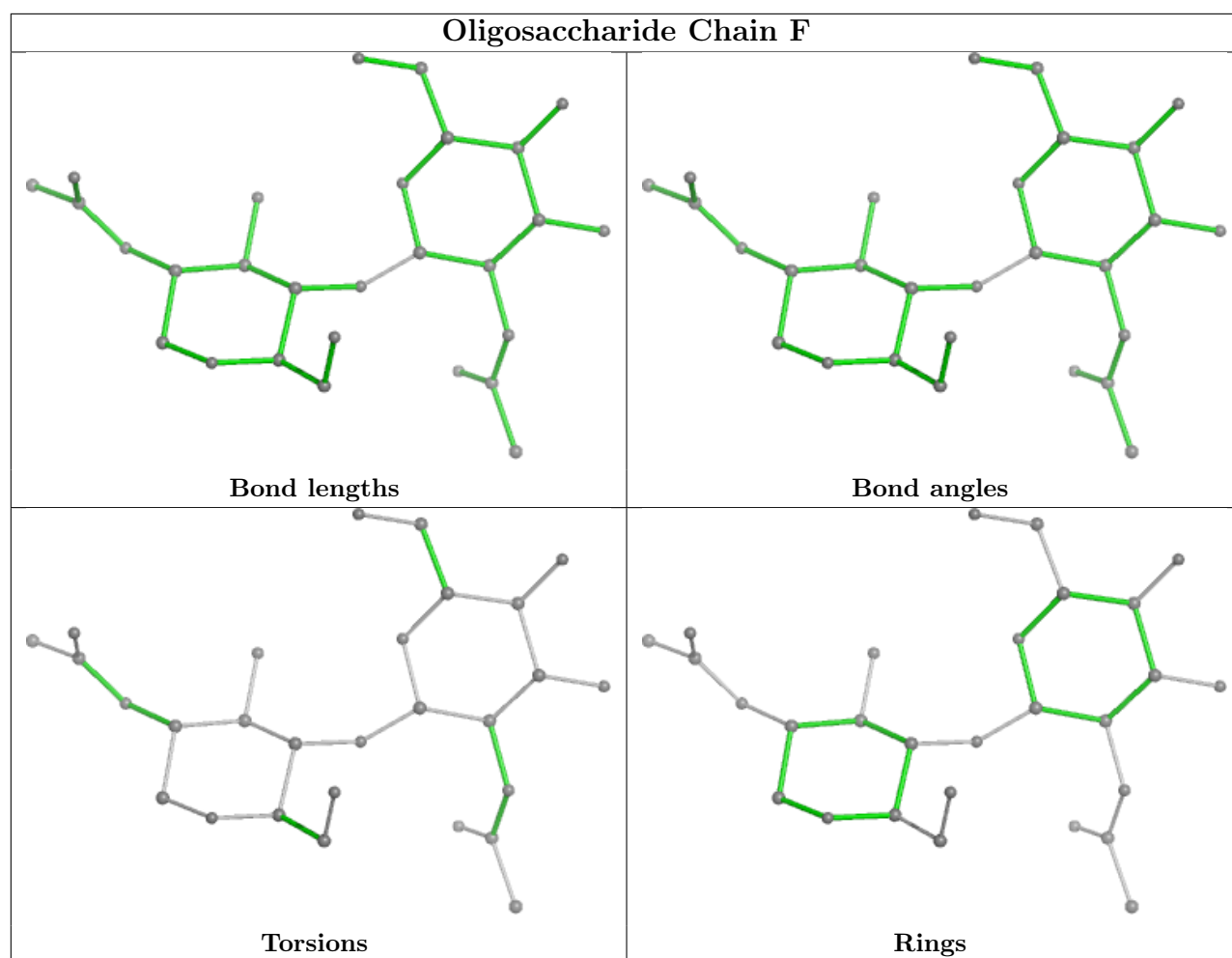
There are no ring outliers.

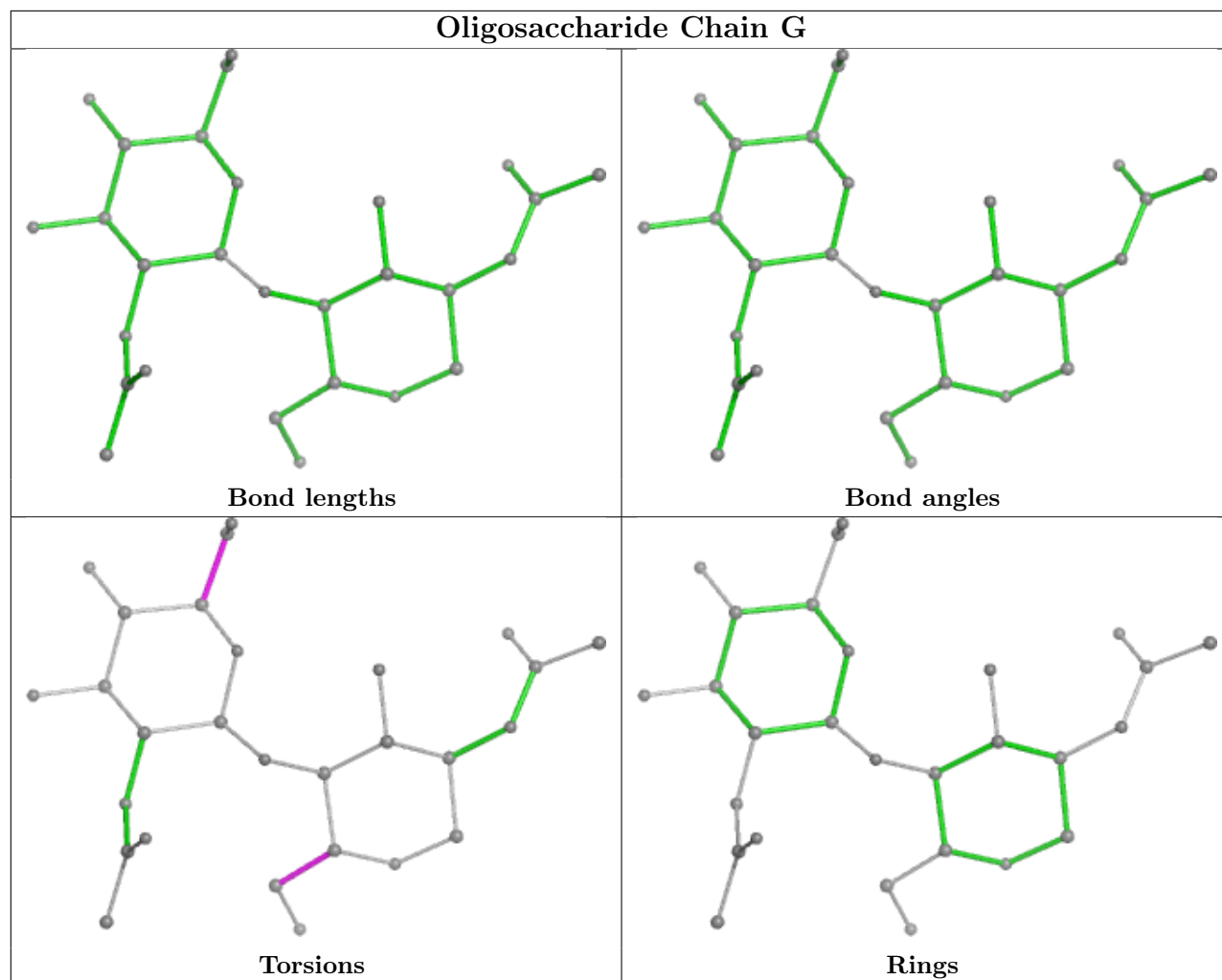
No monomer is involved in short contacts.

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

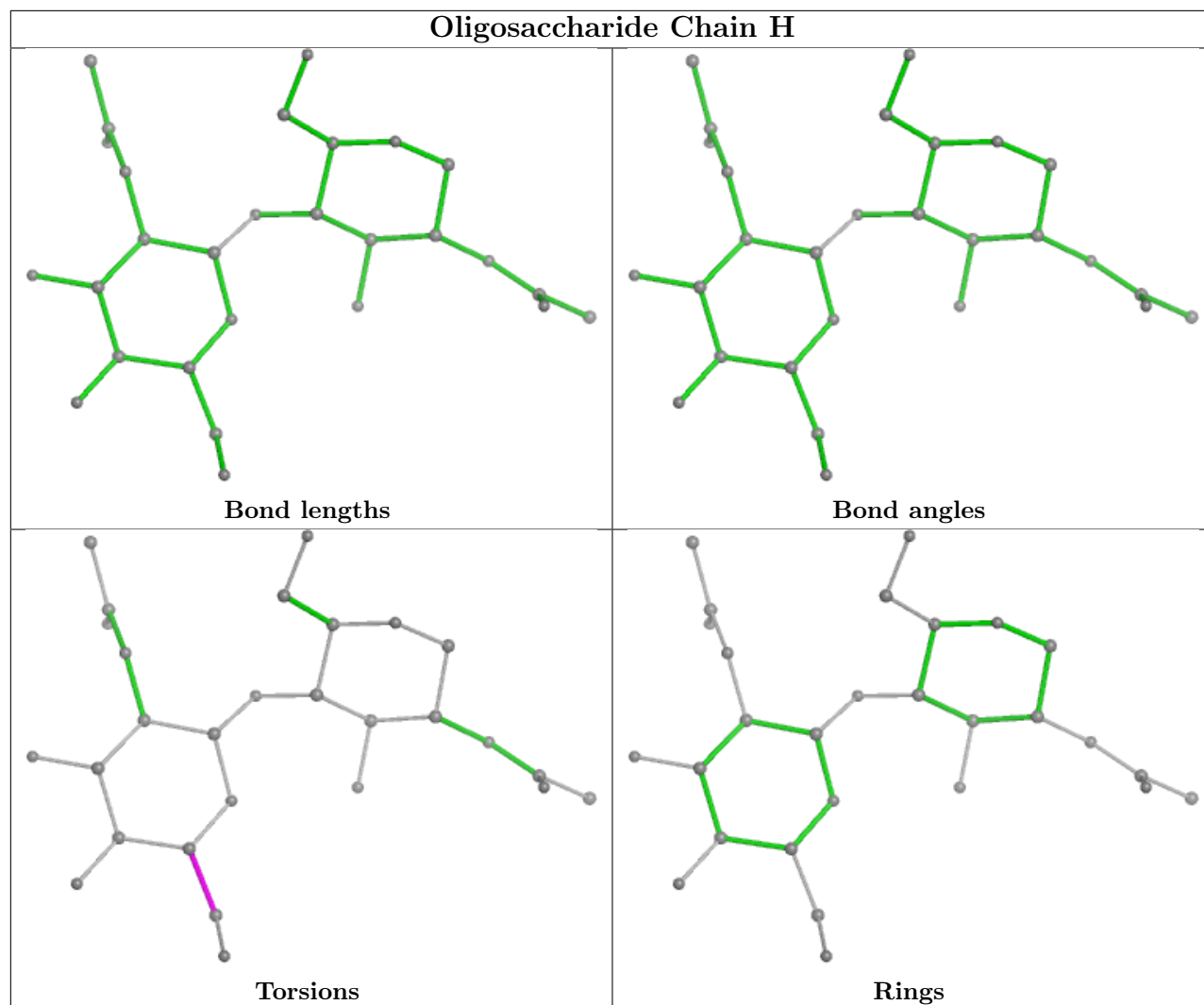


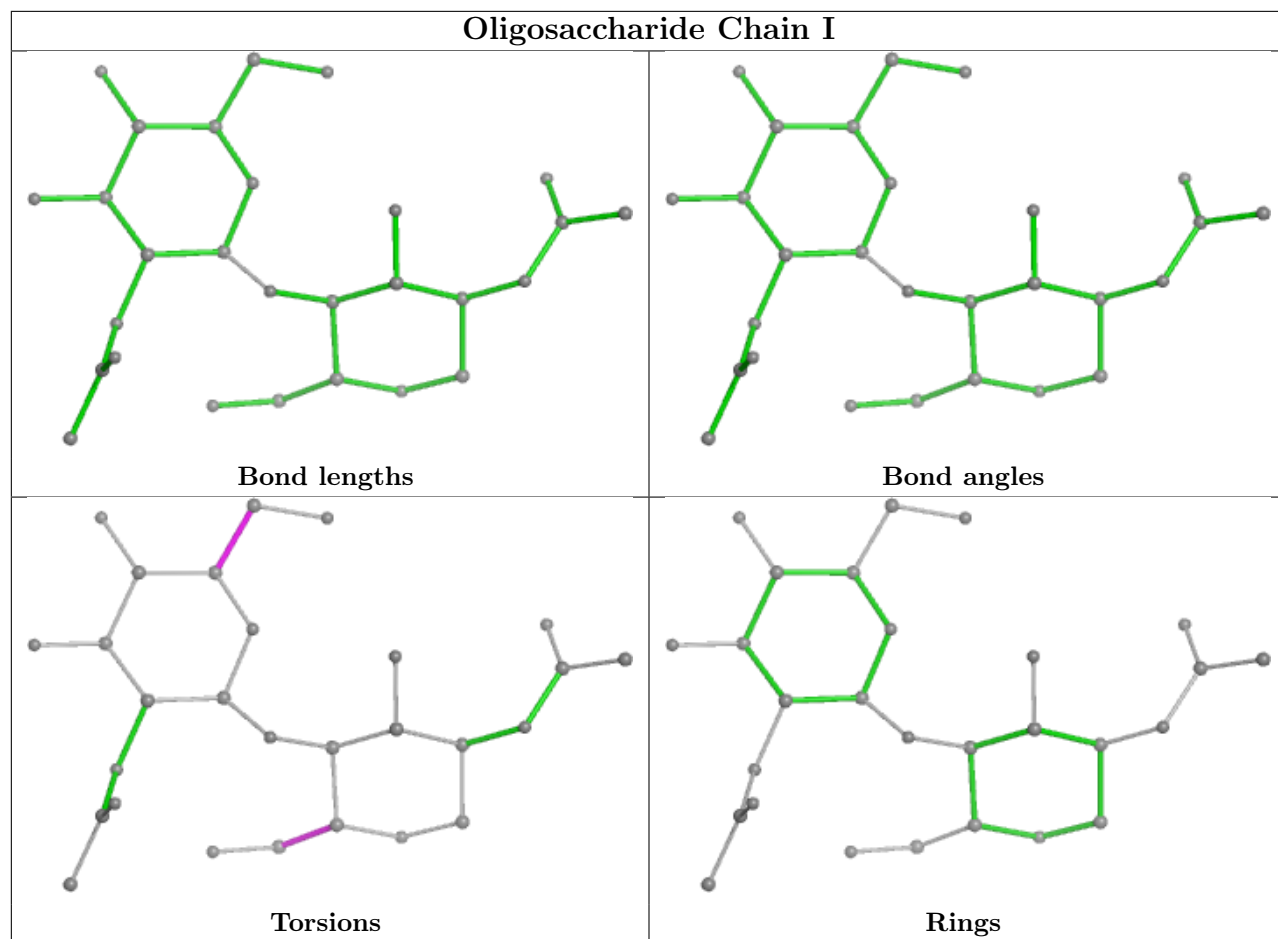


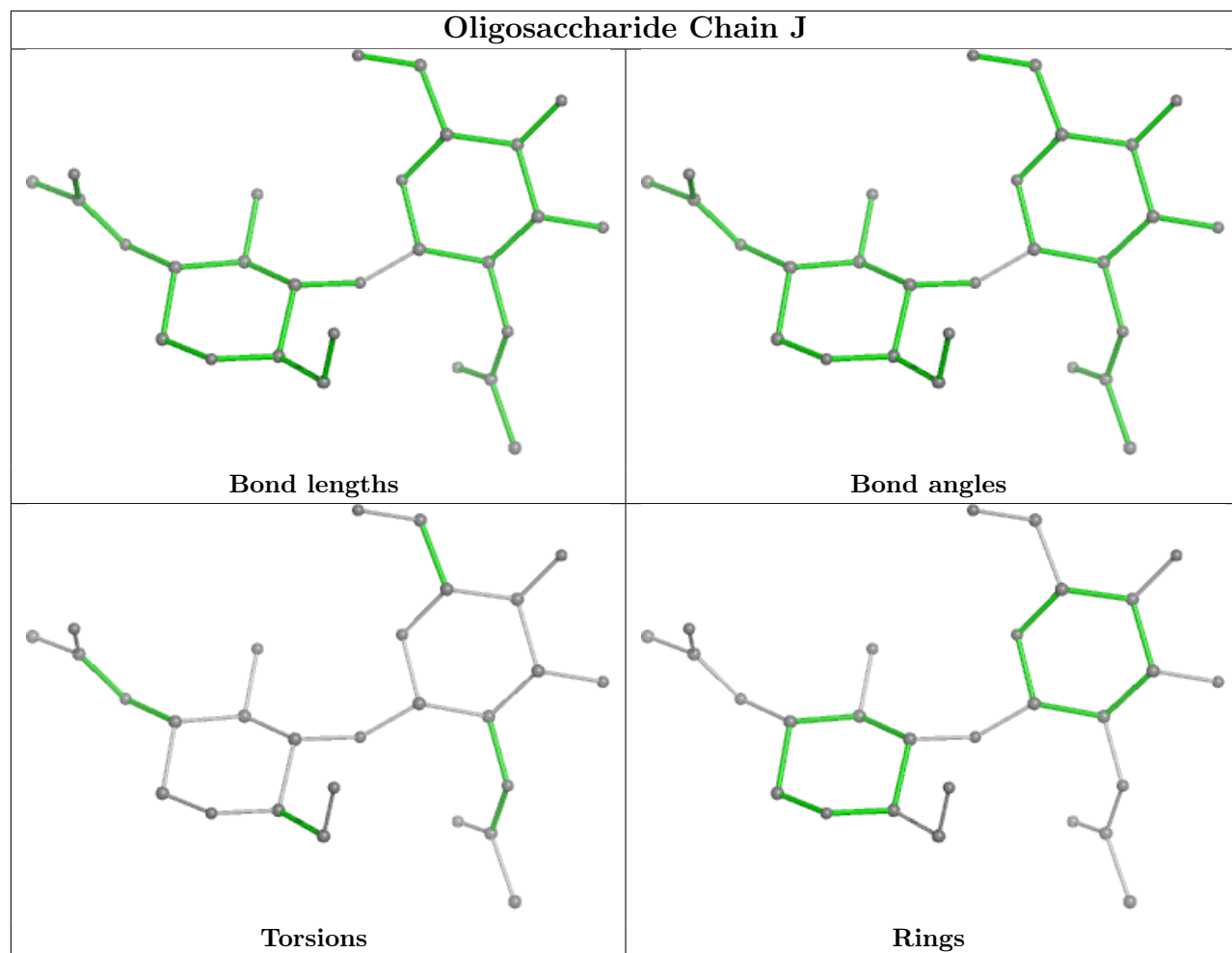


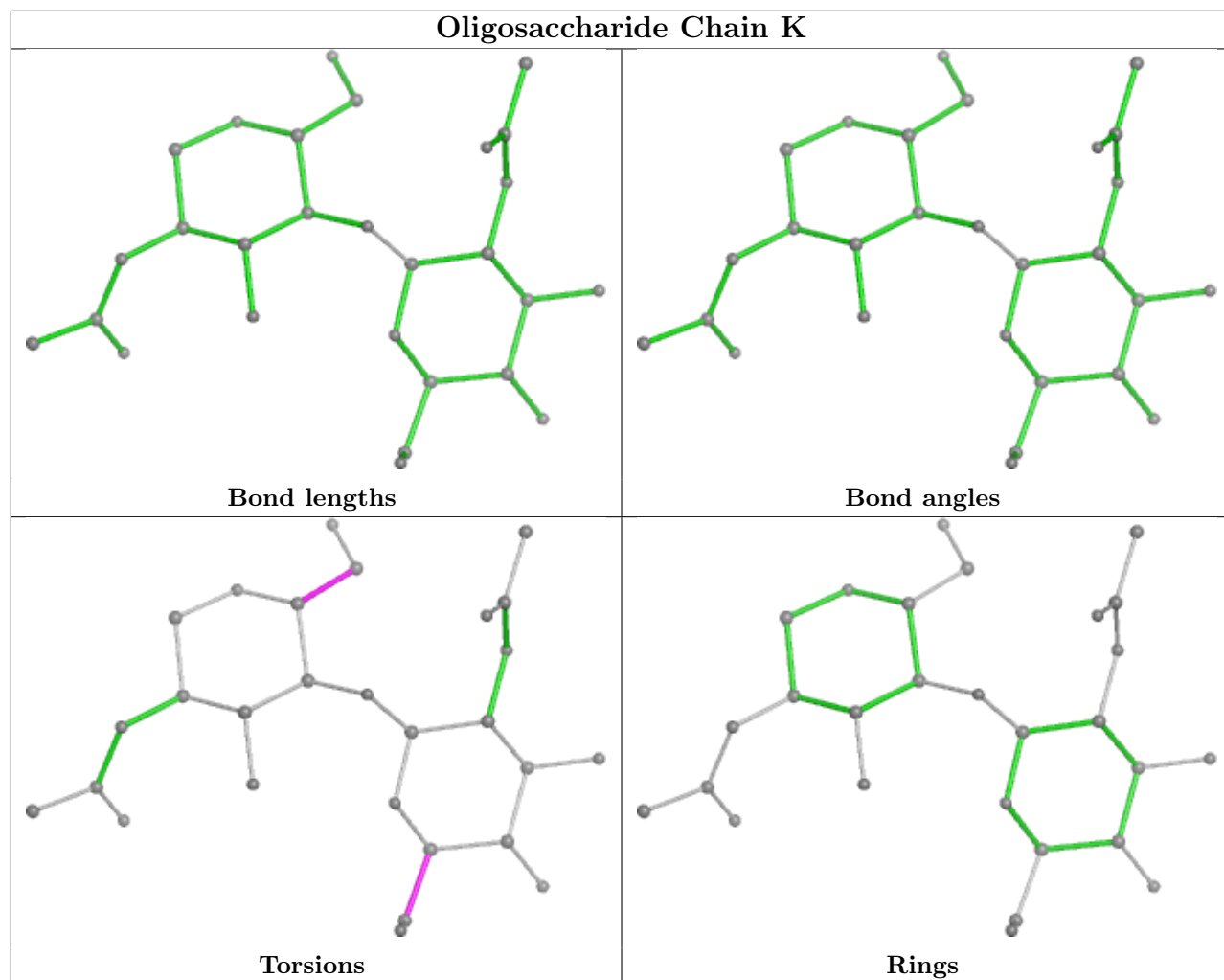


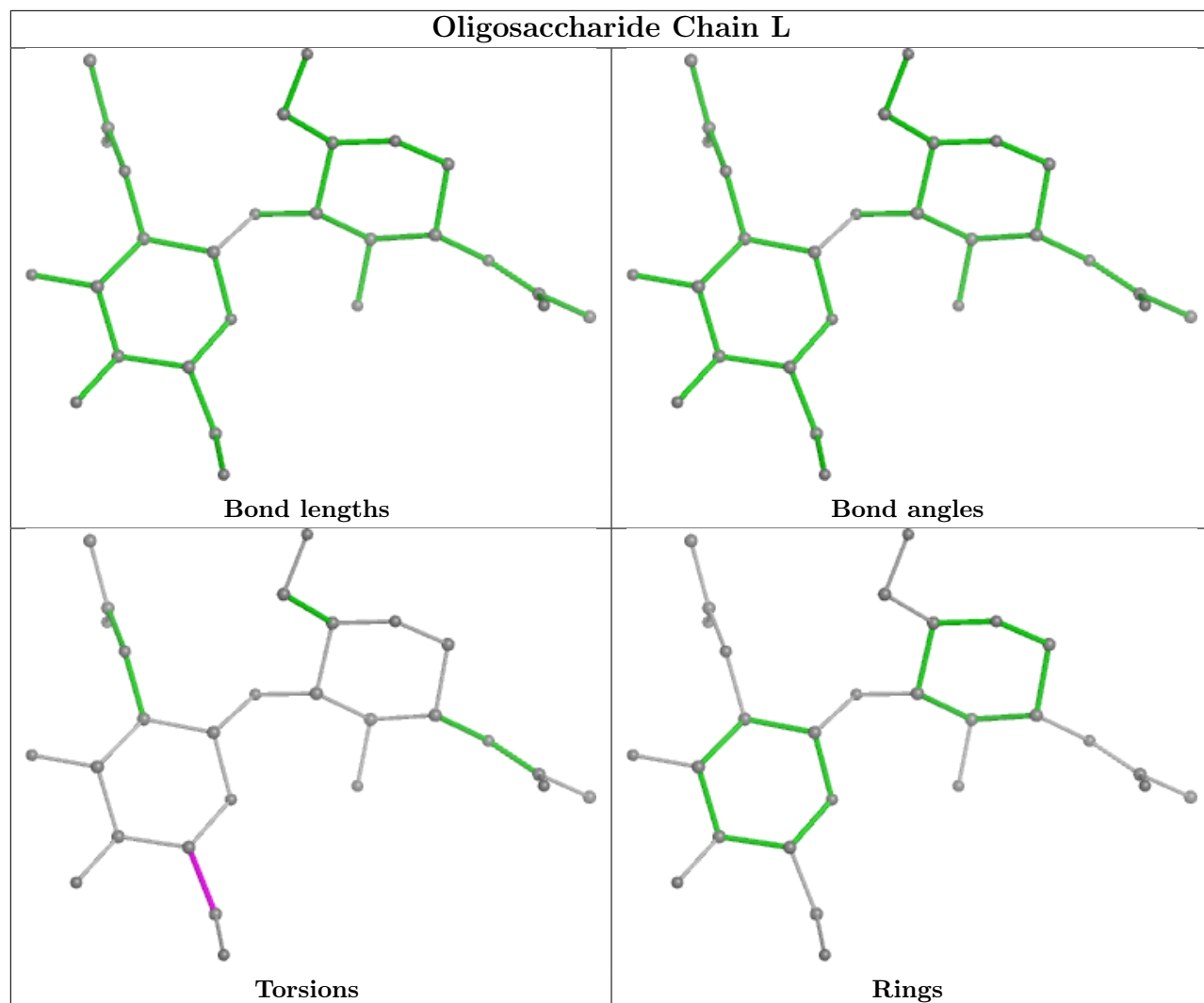


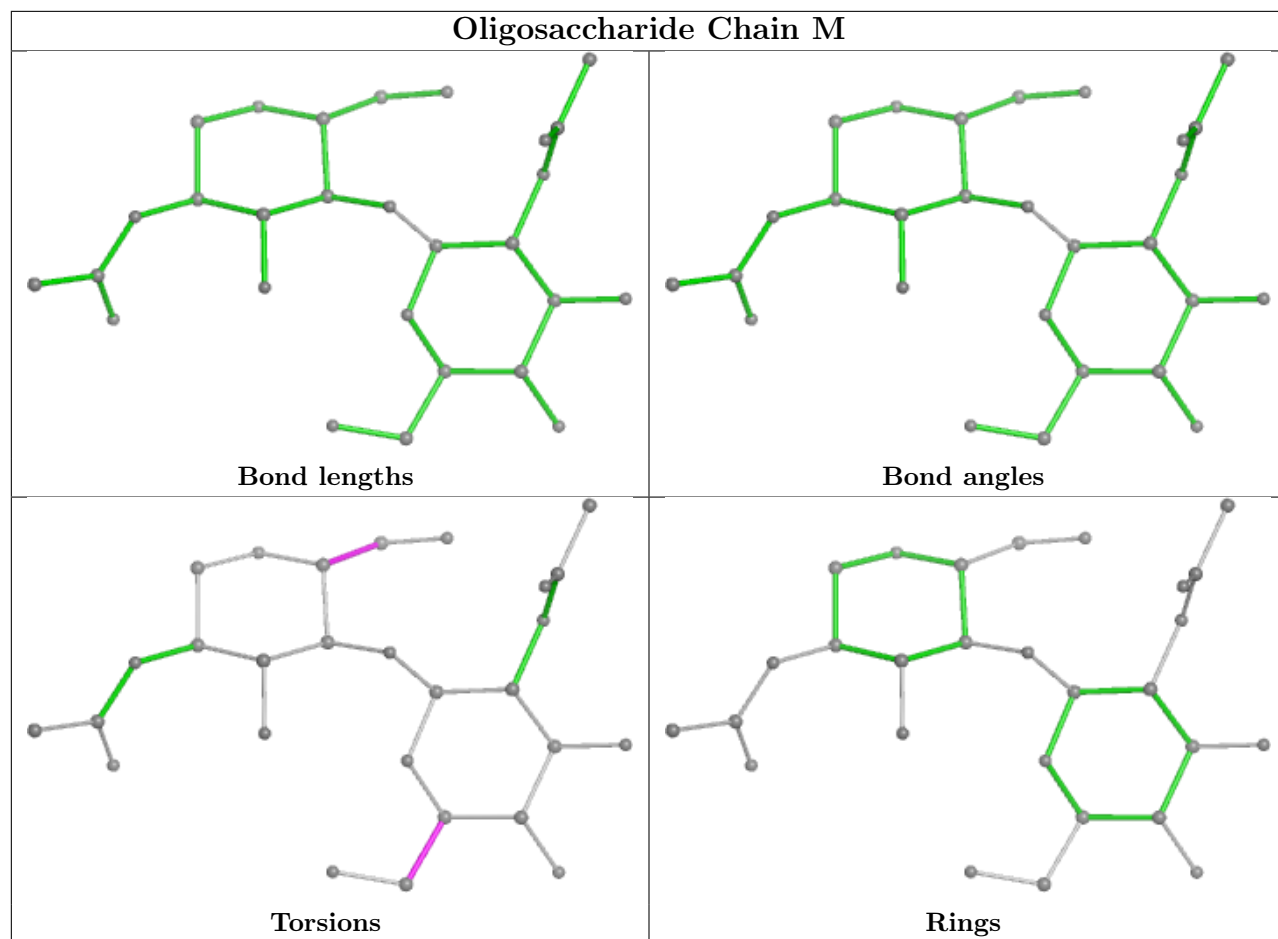


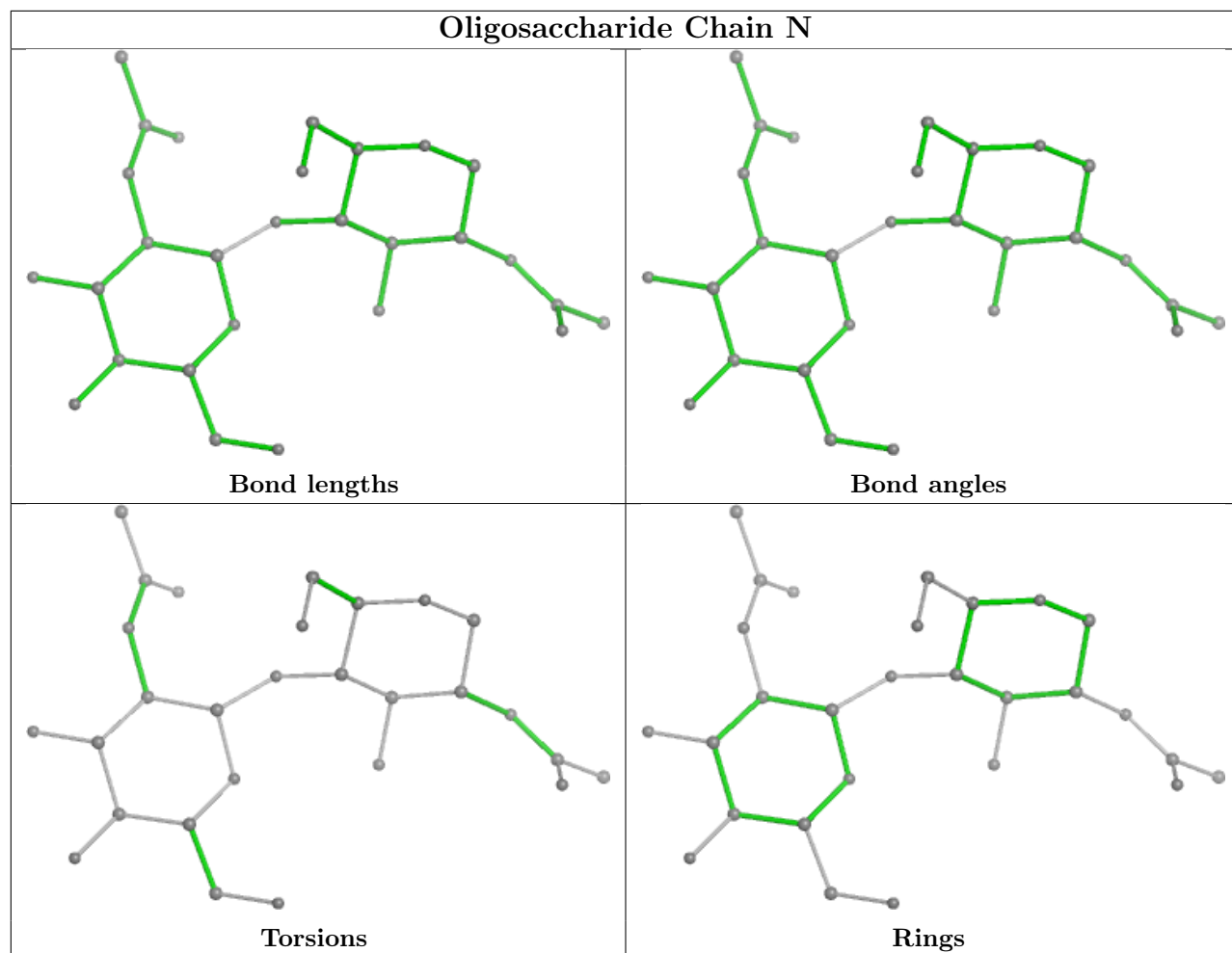


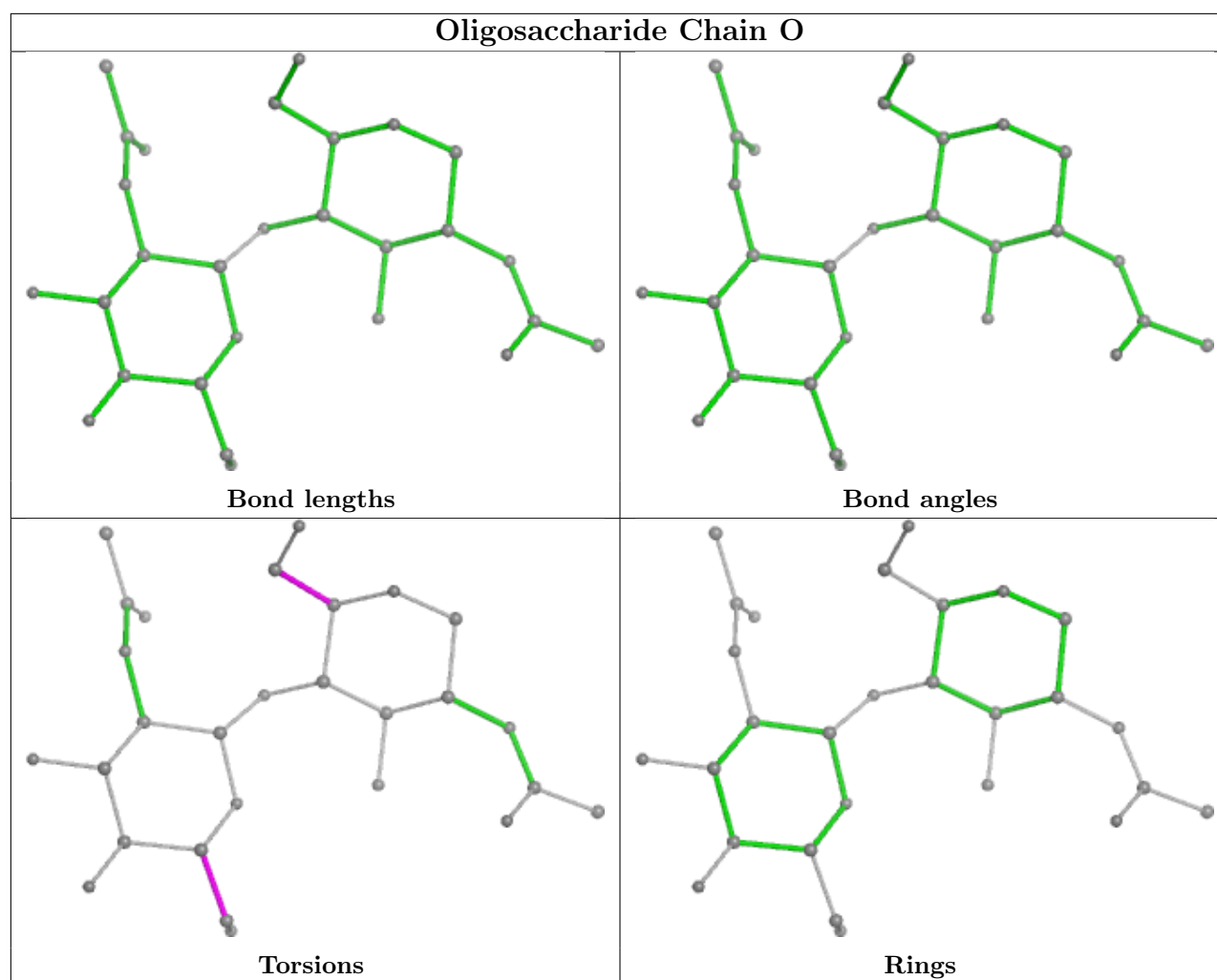












## 5.6 Ligand geometry [i](#)

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	1310	1	14,14,15	0.21	0	17,19,21	0.57	0
3	NAG	B	1304	1	14,14,15	0.20	0	17,19,21	0.57	0
3	NAG	C	1315	1	14,14,15	0.18	0	17,19,21	0.61	0
3	NAG	C	1302	1	14,14,15	0.19	0	17,19,21	0.91	1 (5%)
3	NAG	C	1301	1	14,14,15	0.21	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	B	1308	1	14,14,15	0.30	0	17,19,21	1.41	2 (11%)
3	NAG	C	1309	1	14,14,15	0.39	0	17,19,21	0.51	0
3	NAG	A	1306	1	14,14,15	0.17	0	17,19,21	0.63	0
3	NAG	B	1302	1	14,14,15	0.18	0	17,19,21	0.91	1 (5%)
3	NAG	B	1307	1	14,14,15	0.18	0	17,19,21	0.57	0
3	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.57	0
3	NAG	B	1315	1	14,14,15	0.18	0	17,19,21	0.62	0
3	NAG	C	1303	1	14,14,15	0.35	0	17,19,21	0.62	0
3	NAG	B	1303	1	14,14,15	0.37	0	17,19,21	0.62	0
3	NAG	B	1309	1	14,14,15	0.40	0	17,19,21	0.51	0
3	NAG	C	1304	1	14,14,15	0.20	0	17,19,21	0.58	0
3	NAG	A	1320	1	14,14,15	0.37	0	17,19,21	0.54	0
3	NAG	A	1310	1	14,14,15	0.22	0	17,19,21	0.57	0
3	NAG	C	1320	1	14,14,15	0.37	0	17,19,21	0.54	0
3	NAG	A	1303	1	14,14,15	0.35	0	17,19,21	0.62	0
3	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.62	0
3	NAG	C	1307	1	14,14,15	0.18	0	17,19,21	0.58	0
3	NAG	A	1305	1	14,14,15	0.36	0	17,19,21	0.51	0
3	NAG	A	1302	1	14,14,15	0.18	0	17,19,21	0.91	1 (5%)
3	NAG	B	1306	1	14,14,15	0.18	0	17,19,21	0.62	0
3	NAG	C	1306	1	14,14,15	0.18	0	17,19,21	0.62	0
3	NAG	B	1310	1	14,14,15	0.22	0	17,19,21	0.56	0
3	NAG	A	1301	1	14,14,15	0.23	0	17,19,21	0.62	0
3	NAG	B	1320	1	14,14,15	0.38	0	17,19,21	0.53	0
3	NAG	B	1305	1	14,14,15	0.34	0	17,19,21	0.51	0
3	NAG	A	1315	1	14,14,15	0.18	0	17,19,21	0.61	0
3	NAG	A	1308	1	14,14,15	0.30	0	17,19,21	1.41	2 (11%)
3	NAG	C	1305	1	14,14,15	0.35	0	17,19,21	0.51	0
3	NAG	A	1307	1	14,14,15	0.17	0	17,19,21	0.58	0
3	NAG	A	1309	1	14,14,15	0.39	0	17,19,21	0.51	0
3	NAG	C	1308	1	14,14,15	0.30	0	17,19,21	1.41	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	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1315	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	5/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1315	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1320	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1320	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1303	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	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1320	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1315	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	5/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	C	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	A	1308	NAG	C2-N2-C7	4.52	129.34	122.90
3	B	1308	NAG	C2-N2-C7	4.51	129.32	122.90
3	C	1308	NAG	C2-N2-C7	4.48	129.28	122.90
3	C	1302	NAG	C2-N2-C7	2.81	126.90	122.90
3	B	1302	NAG	C2-N2-C7	2.79	126.88	122.90
3	A	1302	NAG	C2-N2-C7	2.77	126.85	122.90
3	C	1308	NAG	C1-C2-N2	2.33	114.47	110.49
3	B	1308	NAG	C1-C2-N2	2.31	114.43	110.49
3	A	1308	NAG	C1-C2-N2	2.29	114.39	110.49

There are no chirality outliers.

All (81) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
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
3	C	1308	NAG	C8-C7-N2-C2
3	C	1308	NAG	O7-C7-N2-C2
3	A	1307	NAG	O5-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	A	1320	NAG	C4-C5-C6-O6
3	B	1320	NAG	C4-C5-C6-O6
3	C	1320	NAG	C4-C5-C6-O6
3	A	1315	NAG	O5-C5-C6-O6
3	B	1315	NAG	O5-C5-C6-O6
3	C	1315	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	1307	NAG	C4-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	C	1307	NAG	C4-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-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	1320	NAG	C1-C2-N2-C7
3	B	1320	NAG	C1-C2-N2-C7
3	C	1320	NAG	C1-C2-N2-C7
3	A	1308	NAG	C3-C2-N2-C7
3	B	1308	NAG	C3-C2-N2-C7
3	C	1308	NAG	C3-C2-N2-C7
3	A	1303	NAG	C4-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	C	1303	NAG	C4-C5-C6-O6
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	1308	NAG	C1-C2-N2-C7
3	B	1308	NAG	C1-C2-N2-C7
3	C	1308	NAG	C1-C2-N2-C7
3	A	1320	NAG	C3-C2-N2-C7
3	B	1320	NAG	C3-C2-N2-C7
3	C	1320	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

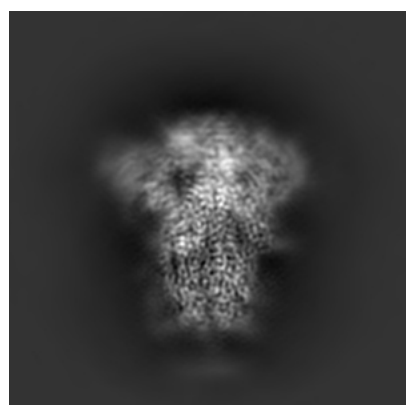
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11330. These allow visual inspection of the internal detail of the map and identification of artifacts.

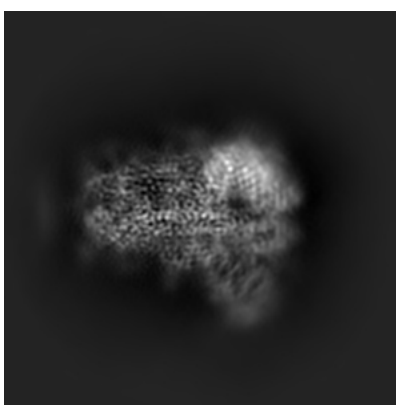
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

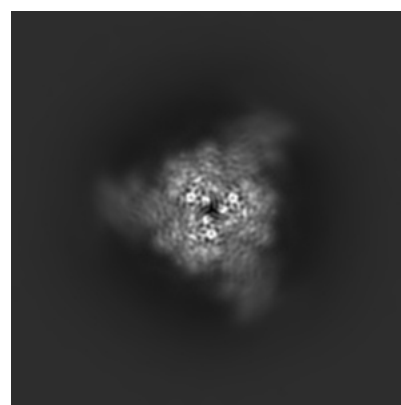
#### 6.1.1 Primary map



X



Y

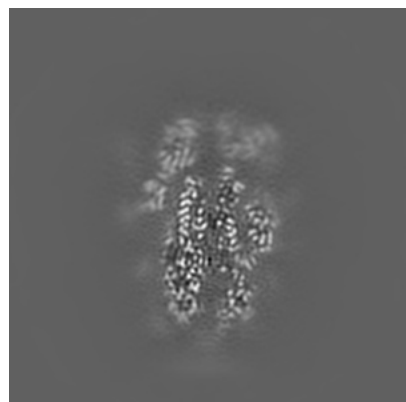


Z

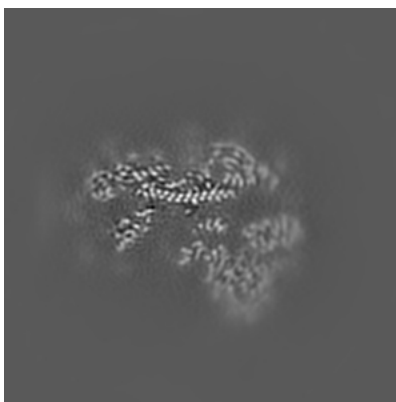
The images above show the map projected in three orthogonal directions.

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

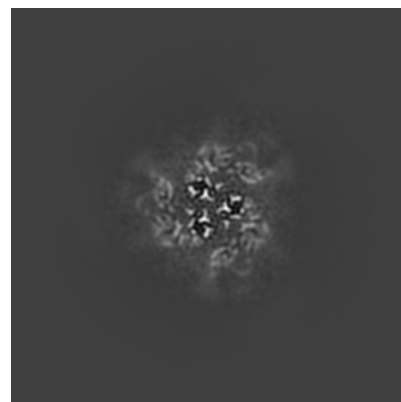
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

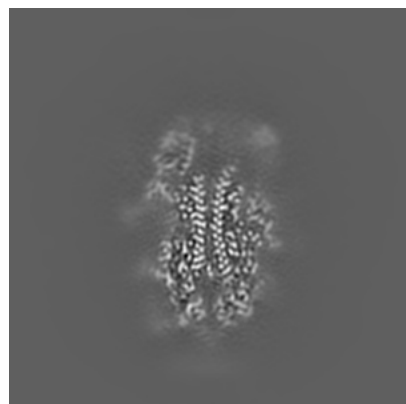


Z Index: 128

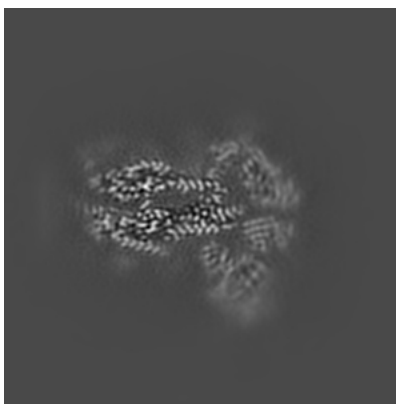
The images above show central slices of the map in three orthogonal directions.

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

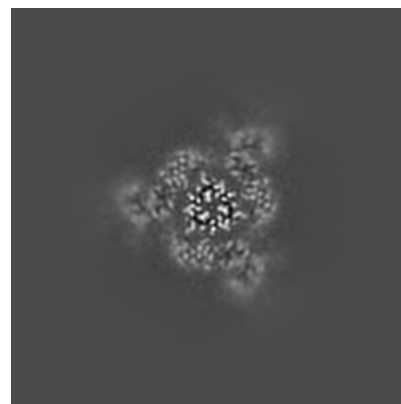
### 6.3.1 Primary map



X Index: 124



Y Index: 137

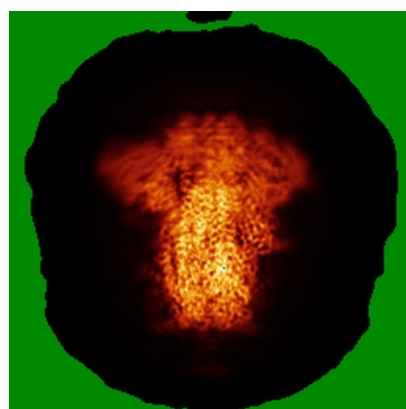


Z Index: 137

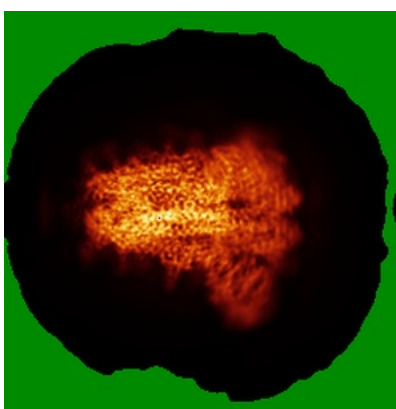
The images above show the largest variance slices of the map in three orthogonal directions.

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

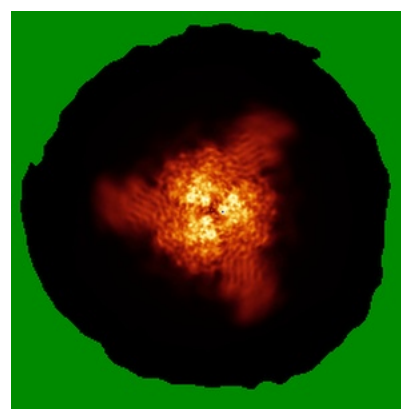
### 6.4.1 Primary map



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 0.0211. 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](#)

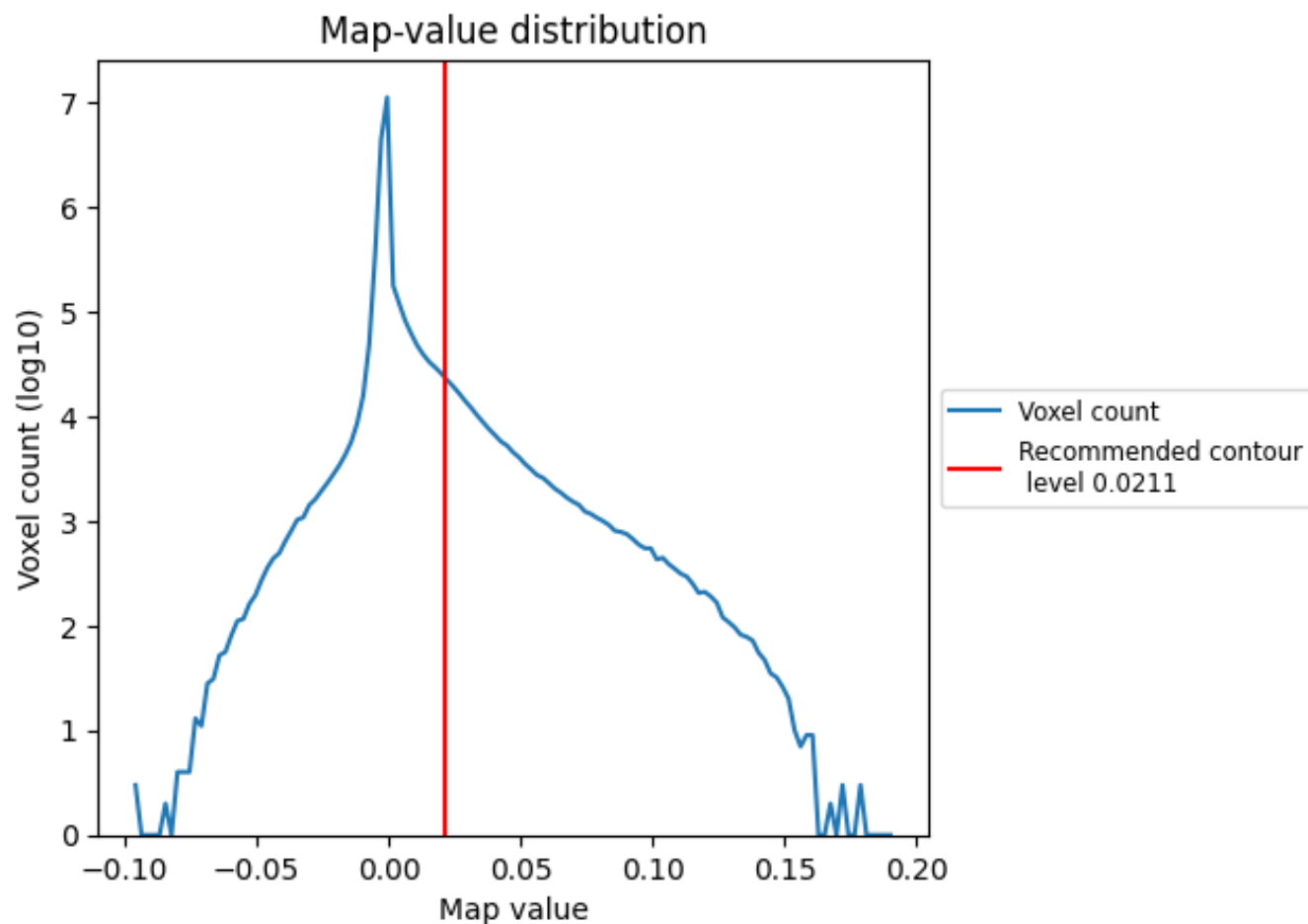
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

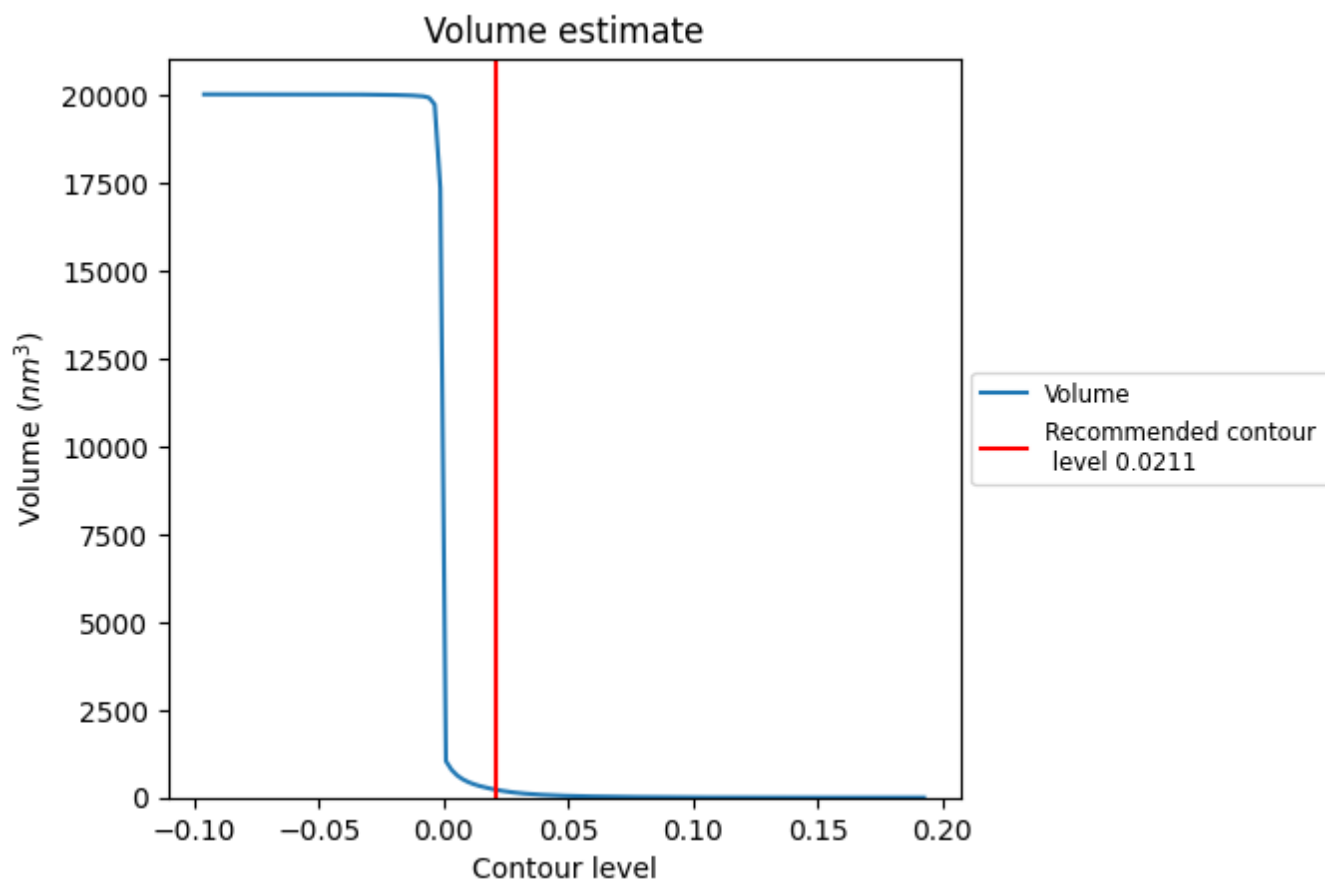
This section contains the results of statistical analysis of the map.

### 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.

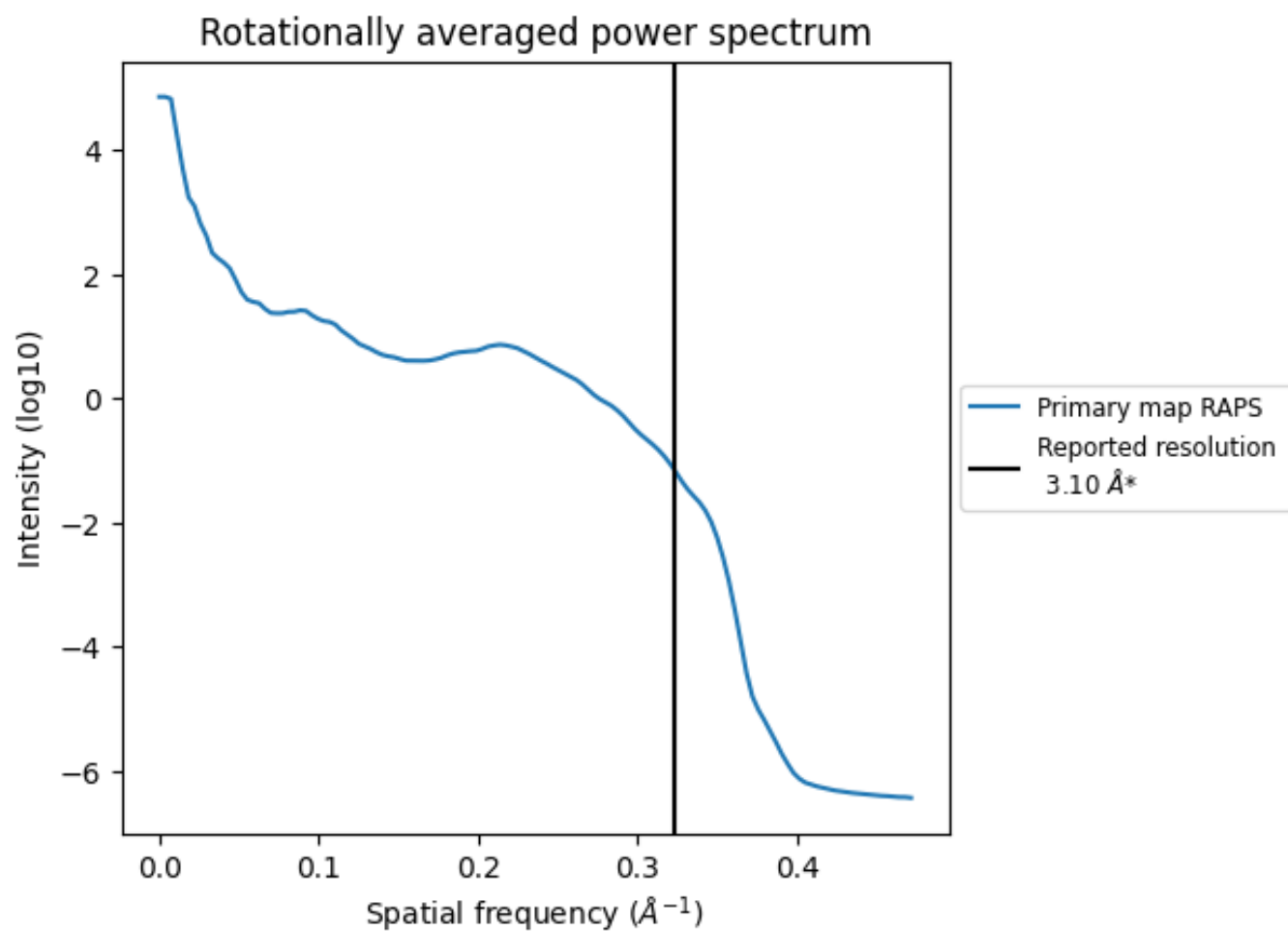
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 221 nm<sup>3</sup>; this corresponds to an approximate mass of 200 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 0.323 Å<sup>-1</sup>

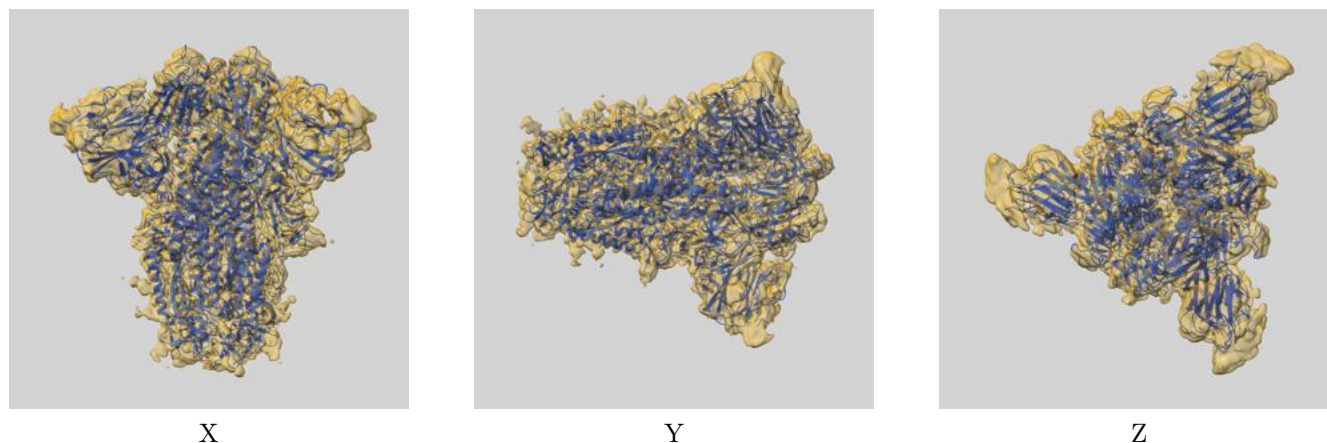
## 8 Fourier-Shell correlation

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

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

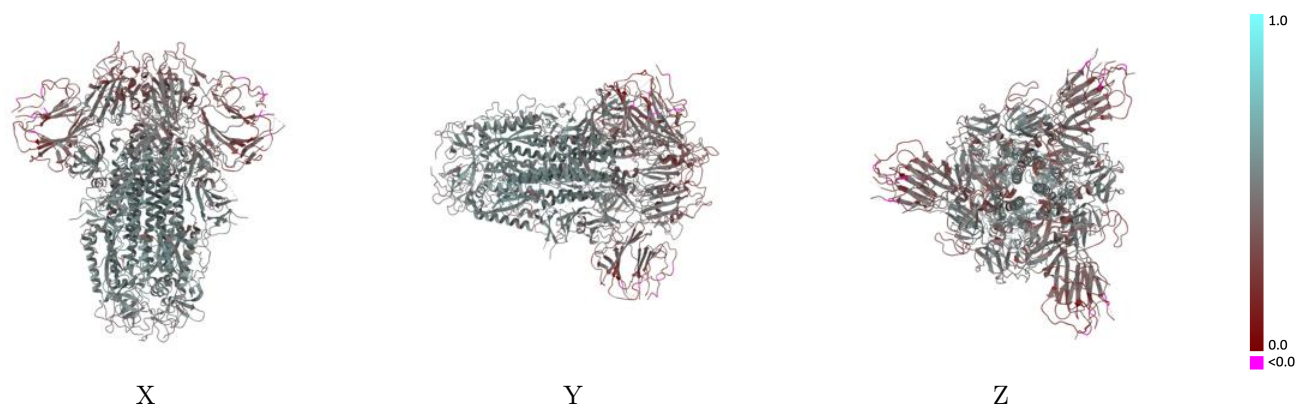
This section contains information regarding the fit between EMDB map EMD-11330 and PDB model 6ZOY. Per-residue inclusion information can be found in section 3 on page 12.

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



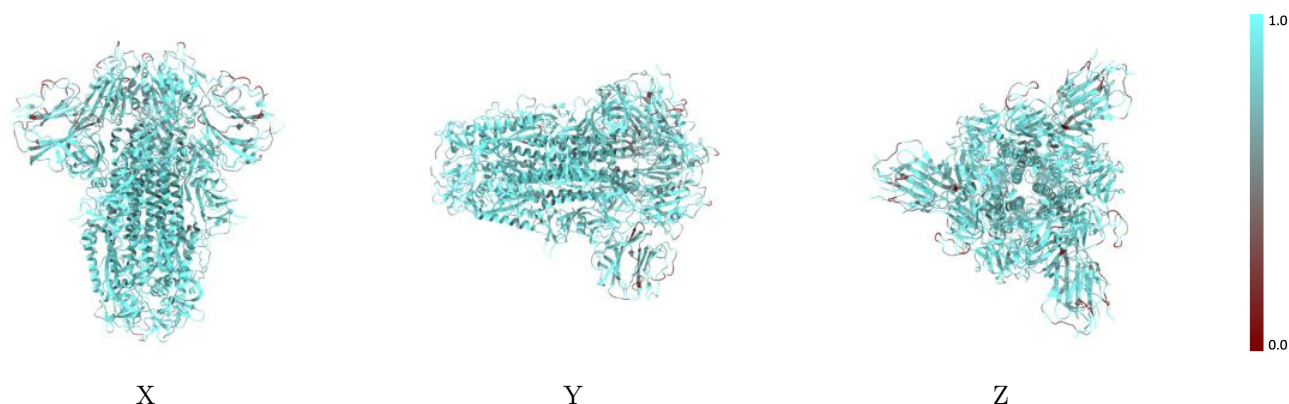
The images above show the 3D surface view of the map at the recommended contour level 0.0211 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



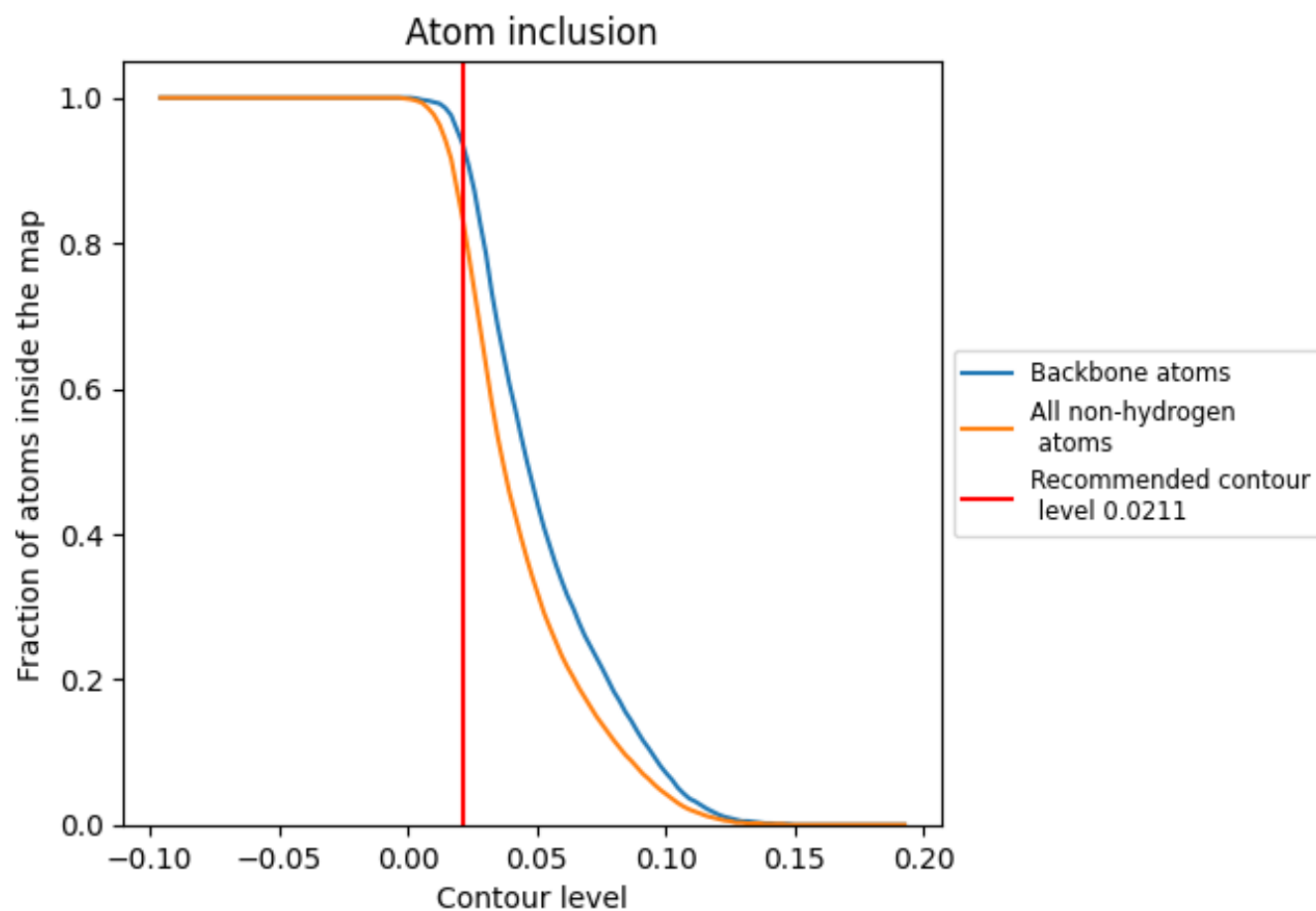
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0211).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 84% 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 (0.0211) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8370</div>	<div><div></div>0.4430</div>
A	<div><div></div>0.8390</div>	<div><div></div>0.4440</div>
B	<div><div></div>0.8370</div>	<div><div></div>0.4440</div>
C	<div><div></div>0.8390</div>	<div><div></div>0.4430</div>
D	<div><div></div>0.8570</div>	<div><div></div>0.5010</div>
E	<div><div></div>0.7500</div>	<div><div></div>0.3750</div>
F	<div><div></div>0.6430</div>	<div><div></div>0.4070</div>
G	<div><div></div>0.6430</div>	<div><div></div>0.3840</div>
H	<div><div></div>0.8210</div>	<div><div></div>0.5040</div>
I	<div><div></div>0.7500</div>	<div><div></div>0.3780</div>
J	<div><div></div>0.6790</div>	<div><div></div>0.4070</div>
K	<div><div></div>0.6430</div>	<div><div></div>0.3860</div>
L	<div><div></div>0.8210</div>	<div><div></div>0.4970</div>
M	<div><div></div>0.7500</div>	<div><div></div>0.3850</div>
N	<div><div></div>0.6790</div>	<div><div></div>0.4100</div>
O	<div><div></div>0.6430</div>	<div><div></div>0.3880</div>

1.0

0.0

<0.0