



## Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 09:14 pm BST

PDB ID : 7Q9I  
EMDB ID : EMD-13870  
Title : Beta-43 fab in complex with SARS-CoV-2 beta-Spike glycoprotein  
Authors : Duyvesteyn, H.M.E.; Ren, J.; Stuart, D.I.  
Deposited on : 2021-11-12  
Resolution : 4.90 Å (reported)  
Based on initial model : 7Q0I

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

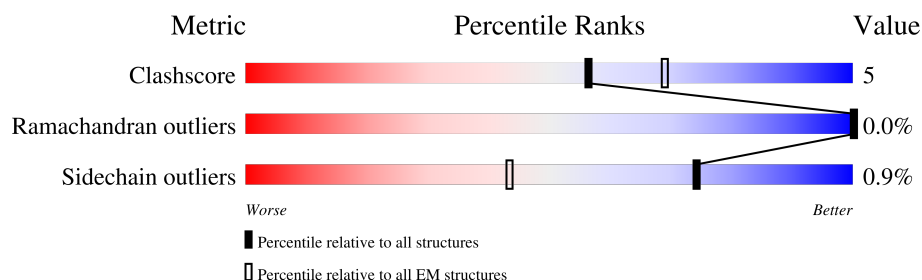
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.90 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	1285	
1	B	1285	
1	C	1285	
2	E	231	
2	H	231	
2	J	231	
3	F	214	
3	K	214	

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Mol	Chain	Length	Quality of chain
3	L	214	
4	D	2	
4	G	2	
4	I	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30966 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	1062	Total	C	N	O	S	0	0
			8290	5294	1381	1577	38		
1	B	1058	Total	C	N	O	S	0	0
			8267	5282	1377	1570	38		
1	C	1059	Total	C	N	O	S	0	0
			8273	5285	1378	1572	38		

There are 291 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	80	ALA	ASP	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	243	ILE	ARG	variant	UNP P0DTC2
A	414	ASN	LYS	variant	UNP P0DTC2
A	481	LYS	GLU	variant	UNP P0DTC2
A	498	TYR	ASN	variant	UNP P0DTC2
A	611	GLY	ASP	variant	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	680	SER	ARG	conflict	UNP P0DTC2
A	682	SER	ARG	conflict	UNP P0DTC2
A	698	VAL	ALA	variant	UNP P0DTC2
A	983	PRO	LYS	conflict	UNP P0DTC2
A	984	PRO	VAL	conflict	UNP P0DTC2
A	1206	GLY	-	expression tag	UNP P0DTC2
A	1207	SER	-	expression tag	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
A	1209	TYR	-	expression tag	UNP P0DTC2
A	1210	ILE	-	expression tag	UNP P0DTC2
A	1211	PRO	-	expression tag	UNP P0DTC2
A	1212	GLU	-	expression tag	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1255	GLY	-	expression tag	UNP P0DTC2
A	1256	SER	-	expression tag	UNP P0DTC2
A	1257	ALA	-	expression tag	UNP P0DTC2
A	1258	TRP	-	expression tag	UNP P0DTC2
A	1259	SER	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	PRO	-	expression tag	UNP P0DTC2
A	1262	GLN	-	expression tag	UNP P0DTC2
A	1263	PHE	-	expression tag	UNP P0DTC2
A	1264	GLU	-	expression tag	UNP P0DTC2
A	1265	LYS	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	SER	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	GLY	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	SER	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	ALA	-	expression tag	UNP P0DTC2
A	1278	TRP	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	HIS	-	expression tag	UNP P0DTC2
A	1281	PRO	-	expression tag	UNP P0DTC2
A	1282	GLN	-	expression tag	UNP P0DTC2
A	1283	PHE	-	expression tag	UNP P0DTC2
A	1284	GLU	-	expression tag	UNP P0DTC2
A	1285	LYS	-	expression tag	UNP P0DTC2
B	18	PHE	LEU	variant	UNP P0DTC2
B	80	ALA	ASP	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	243	ILE	ARG	variant	UNP P0DTC2
B	414	ASN	LYS	variant	UNP P0DTC2
B	481	LYS	GLU	variant	UNP P0DTC2
B	498	TYR	ASN	variant	UNP P0DTC2
B	611	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	679	GLY	ARG	conflict	UNP P0DTC2
B	680	SER	ARG	conflict	UNP P0DTC2
B	682	SER	ARG	conflict	UNP P0DTC2
B	698	VAL	ALA	variant	UNP P0DTC2
B	983	PRO	LYS	conflict	UNP P0DTC2
B	984	PRO	VAL	conflict	UNP P0DTC2
B	1206	GLY	-	expression tag	UNP P0DTC2
B	1207	SER	-	expression tag	UNP P0DTC2
B	1208	GLY	-	expression tag	UNP P0DTC2
B	1209	TYR	-	expression tag	UNP P0DTC2
B	1210	ILE	-	expression tag	UNP P0DTC2
B	1211	PRO	-	expression tag	UNP P0DTC2
B	1212	GLU	-	expression tag	UNP P0DTC2
B	1213	ALA	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	ARG	-	expression tag	UNP P0DTC2
B	1216	ASP	-	expression tag	UNP P0DTC2
B	1217	GLY	-	expression tag	UNP P0DTC2
B	1218	GLN	-	expression tag	UNP P0DTC2
B	1219	ALA	-	expression tag	UNP P0DTC2
B	1220	TYR	-	expression tag	UNP P0DTC2
B	1221	VAL	-	expression tag	UNP P0DTC2
B	1222	ARG	-	expression tag	UNP P0DTC2
B	1223	LYS	-	expression tag	UNP P0DTC2
B	1224	ASP	-	expression tag	UNP P0DTC2
B	1225	GLY	-	expression tag	UNP P0DTC2
B	1226	GLU	-	expression tag	UNP P0DTC2
B	1227	TRP	-	expression tag	UNP P0DTC2
B	1228	VAL	-	expression tag	UNP P0DTC2
B	1229	LEU	-	expression tag	UNP P0DTC2
B	1230	LEU	-	expression tag	UNP P0DTC2
B	1231	SER	-	expression tag	UNP P0DTC2
B	1232	THR	-	expression tag	UNP P0DTC2
B	1233	PHE	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	ARG	-	expression tag	UNP P0DTC2
B	1237	SER	-	expression tag	UNP P0DTC2
B	1238	LEU	-	expression tag	UNP P0DTC2
B	1239	GLU	-	expression tag	UNP P0DTC2
B	1240	VAL	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1242	PHE	-	expression tag	UNP P0DTC2
B	1243	GLN	-	expression tag	UNP P0DTC2
B	1244	GLY	-	expression tag	UNP P0DTC2
B	1245	PRO	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
B	1248	HIS	-	expression tag	UNP P0DTC2
B	1249	HIS	-	expression tag	UNP P0DTC2
B	1250	HIS	-	expression tag	UNP P0DTC2
B	1251	HIS	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	HIS	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	GLY	-	expression tag	UNP P0DTC2
B	1256	SER	-	expression tag	UNP P0DTC2
B	1257	ALA	-	expression tag	UNP P0DTC2
B	1258	TRP	-	expression tag	UNP P0DTC2
B	1259	SER	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	PRO	-	expression tag	UNP P0DTC2
B	1262	GLN	-	expression tag	UNP P0DTC2
B	1263	PHE	-	expression tag	UNP P0DTC2
B	1264	GLU	-	expression tag	UNP P0DTC2
B	1265	LYS	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	SER	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	GLY	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	SER	-	expression tag	UNP P0DTC2
B	1274	GLY	-	expression tag	UNP P0DTC2
B	1275	GLY	-	expression tag	UNP P0DTC2
B	1276	SER	-	expression tag	UNP P0DTC2
B	1277	ALA	-	expression tag	UNP P0DTC2
B	1278	TRP	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	HIS	-	expression tag	UNP P0DTC2
B	1281	PRO	-	expression tag	UNP P0DTC2
B	1282	GLN	-	expression tag	UNP P0DTC2
B	1283	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1284	GLU	-	expression tag	UNP P0DTC2
B	1285	LYS	-	expression tag	UNP P0DTC2
C	18	PHE	LEU	variant	UNP P0DTC2
C	80	ALA	ASP	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	243	ILE	ARG	variant	UNP P0DTC2
C	414	ASN	LYS	variant	UNP P0DTC2
C	481	LYS	GLU	variant	UNP P0DTC2
C	498	TYR	ASN	variant	UNP P0DTC2
C	611	GLY	ASP	variant	UNP P0DTC2
C	679	GLY	ARG	conflict	UNP P0DTC2
C	680	SER	ARG	conflict	UNP P0DTC2
C	682	SER	ARG	conflict	UNP P0DTC2
C	698	VAL	ALA	variant	UNP P0DTC2
C	983	PRO	LYS	conflict	UNP P0DTC2
C	984	PRO	VAL	conflict	UNP P0DTC2
C	1206	GLY	-	expression tag	UNP P0DTC2
C	1207	SER	-	expression tag	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
C	1209	TYR	-	expression tag	UNP P0DTC2
C	1210	ILE	-	expression tag	UNP P0DTC2
C	1211	PRO	-	expression tag	UNP P0DTC2
C	1212	GLU	-	expression tag	UNP P0DTC2
C	1213	ALA	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	ARG	-	expression tag	UNP P0DTC2
C	1216	ASP	-	expression tag	UNP P0DTC2
C	1217	GLY	-	expression tag	UNP P0DTC2
C	1218	GLN	-	expression tag	UNP P0DTC2
C	1219	ALA	-	expression tag	UNP P0DTC2
C	1220	TYR	-	expression tag	UNP P0DTC2
C	1221	VAL	-	expression tag	UNP P0DTC2
C	1222	ARG	-	expression tag	UNP P0DTC2
C	1223	LYS	-	expression tag	UNP P0DTC2
C	1224	ASP	-	expression tag	UNP P0DTC2
C	1225	GLY	-	expression tag	UNP P0DTC2
C	1226	GLU	-	expression tag	UNP P0DTC2
C	1227	TRP	-	expression tag	UNP P0DTC2
C	1228	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1229	LEU	-	expression tag	UNP P0DTC2
C	1230	LEU	-	expression tag	UNP P0DTC2
C	1231	SER	-	expression tag	UNP P0DTC2
C	1232	THR	-	expression tag	UNP P0DTC2
C	1233	PHE	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	ARG	-	expression tag	UNP P0DTC2
C	1237	SER	-	expression tag	UNP P0DTC2
C	1238	LEU	-	expression tag	UNP P0DTC2
C	1239	GLU	-	expression tag	UNP P0DTC2
C	1240	VAL	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	PHE	-	expression tag	UNP P0DTC2
C	1243	GLN	-	expression tag	UNP P0DTC2
C	1244	GLY	-	expression tag	UNP P0DTC2
C	1245	PRO	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2
C	1248	HIS	-	expression tag	UNP P0DTC2
C	1249	HIS	-	expression tag	UNP P0DTC2
C	1250	HIS	-	expression tag	UNP P0DTC2
C	1251	HIS	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	HIS	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	GLY	-	expression tag	UNP P0DTC2
C	1256	SER	-	expression tag	UNP P0DTC2
C	1257	ALA	-	expression tag	UNP P0DTC2
C	1258	TRP	-	expression tag	UNP P0DTC2
C	1259	SER	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	PRO	-	expression tag	UNP P0DTC2
C	1262	GLN	-	expression tag	UNP P0DTC2
C	1263	PHE	-	expression tag	UNP P0DTC2
C	1264	GLU	-	expression tag	UNP P0DTC2
C	1265	LYS	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	GLY	-	expression tag	UNP P0DTC2
C	1269	SER	-	expression tag	UNP P0DTC2
C	1270	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1271	GLY	-	expression tag	UNP P0DTC2
C	1272	GLY	-	expression tag	UNP P0DTC2
C	1273	SER	-	expression tag	UNP P0DTC2
C	1274	GLY	-	expression tag	UNP P0DTC2
C	1275	GLY	-	expression tag	UNP P0DTC2
C	1276	SER	-	expression tag	UNP P0DTC2
C	1277	ALA	-	expression tag	UNP P0DTC2
C	1278	TRP	-	expression tag	UNP P0DTC2
C	1279	SER	-	expression tag	UNP P0DTC2
C	1280	HIS	-	expression tag	UNP P0DTC2
C	1281	PRO	-	expression tag	UNP P0DTC2
C	1282	GLN	-	expression tag	UNP P0DTC2
C	1283	PHE	-	expression tag	UNP P0DTC2
C	1284	GLU	-	expression tag	UNP P0DTC2
C	1285	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Beta-43 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	126	Total	C	N	O	S	0	0
			983	626	166	185	6		
2	E	126	Total	C	N	O	S	0	0
			983	626	166	185	6		
2	J	126	Total	C	N	O	S	0	0
			983	626	166	185	6		

- Molecule 3 is a protein called Beta-43 light chain.

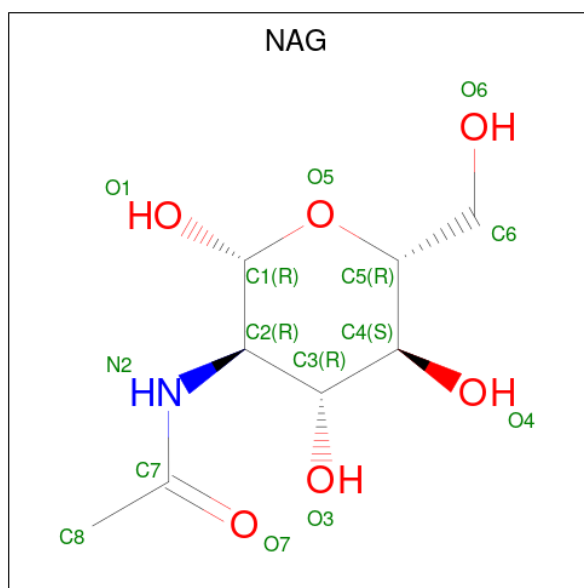
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	108	Total	C	N	O	S	0	0
			815	510	137	166	2		
3	F	108	Total	C	N	O	S	0	0
			815	510	137	166	2		
3	K	108	Total	C	N	O	S	0	0
			815	510	137	166	2		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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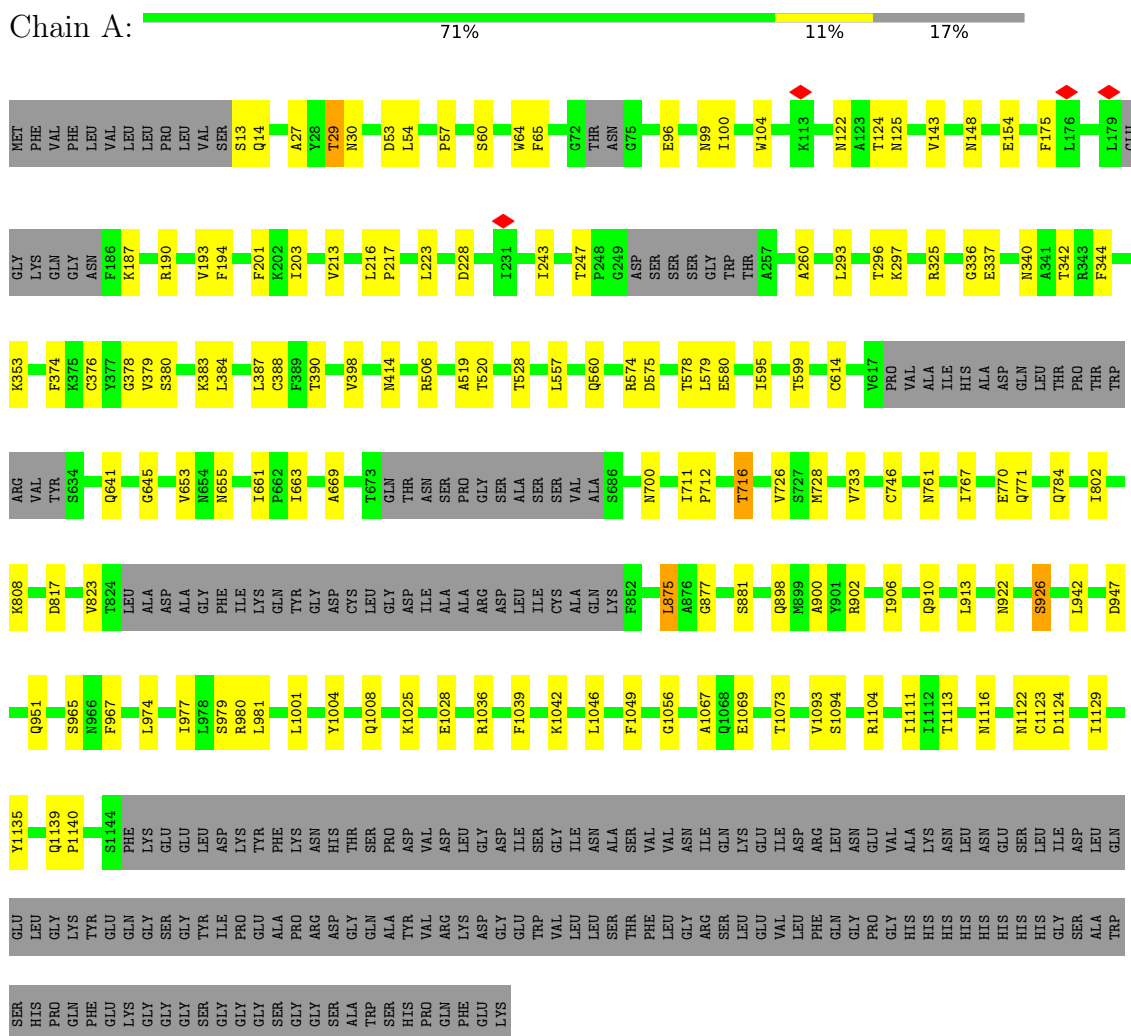
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

### 3 Residue-property plots

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

#### • Molecule 1: Spike glycoprotein



#### • Molecule 1: Spike glycoprotein













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

Chain I:  100%



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

Chain M:  100%



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

Chain N:  100%



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

Chain O:  100%



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

Chain P:  100%



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

Chain Q:  100%



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

Chain R:  100%



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

Chain S:  100%



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

Chain T:  50% 50%



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

Chain U:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	89350	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.440	Depositor
Minimum map value	-0.744	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	464.8, 464.8, 464.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.66, 1.66, 1.66	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	0.29	0/8483	0.49	0/11544
1	B	0.29	0/8460	0.49	0/11513
1	C	0.29	0/8466	0.48	0/11521
2	E	0.27	0/1010	0.50	0/1369
2	H	0.27	0/1010	0.50	0/1369
2	J	0.27	0/1010	0.50	0/1369
3	F	0.26	0/836	0.49	0/1144
3	K	0.26	0/836	0.49	0/1144
3	L	0.26	0/836	0.48	0/1144
All	All	0.28	0/30947	0.49	0/42117

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8290	0	8072	90	0
1	B	8267	0	8052	86	0
1	C	8273	0	8058	86	0
2	E	983	0	919	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	983	0	919	8	0
2	J	983	0	919	8	0
3	F	815	0	773	12	0
3	K	815	0	773	12	0
3	L	815	0	773	10	0
4	D	28	0	25	0	0
4	G	28	0	25	0	0
4	I	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
5	A	140	0	130	0	0
5	B	140	0	130	1	0
5	C	126	0	117	0	0
All	All	30966	0	29935	284	0

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

All (284) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLY:HA2	1:B:970:ILE:HG21	1.62	0.82
1:B:977:ILE:HG23	1:B:981:LEU:HD12	1.64	0.79
1:B:567:ALA:HB1	1:C:960:VAL:HG11	1.72	0.72
1:C:1113:THR:HG22	1:C:1135:TYR:HB3	1.74	0.69
1:C:143:VAL:HG12	1:C:154:GLU:HB3	1.75	0.69
1:B:143:VAL:HG12	1:B:154:GLU:HB3	1.74	0.68
1:A:143:VAL:HG12	1:A:154:GLU:HB3	1.75	0.68
1:C:663:ILE:HD11	1:C:669:ALA:HB2	1.74	0.67
1:B:970:ILE:HD12	1:B:980:ARG:NH2	2.09	0.67
1:C:1111:ILE:O	1:C:1116:ASN:ND2	2.28	0.67
1:C:653:VAL:HG12	1:C:655:ASN:H	1.60	0.66
1:C:1025:LYS:NZ	1:C:1039:PHE:O	2.27	0.66
1:B:1088:ARG:NH1	1:B:1117:THR:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:ARG:O	1:C:380:SER:N	2.28	0.66
1:A:325:ARG:NH2	1:A:528:THR:O	2.29	0.65
1:A:1025:LYS:NZ	1:A:1039:PHE:O	2.30	0.65
1:A:947:ASP:OD2	1:A:951:GLN:NE2	2.30	0.64
1:B:560:GLN:O	1:B:574:ARG:NH1	2.30	0.64
1:A:378:GLY:HA2	1:B:970:ILE:HD13	1.80	0.63
1:B:900:ALA:HB1	1:B:910:GLN:HB2	1.81	0.63
1:A:653:VAL:HG12	1:A:655:ASN:H	1.64	0.62
1:B:1025:LYS:NZ	1:B:1039:PHE:O	2.32	0.62
1:B:1111:ILE:O	1:B:1116:ASN:ND2	2.32	0.62
1:A:53:ASP:OD1	1:A:54:LEU:N	2.30	0.62
1:A:143:VAL:HG12	1:A:154:GLU:CB	2.31	0.61
1:B:143:VAL:HG12	1:B:154:GLU:CB	2.30	0.61
1:C:143:VAL:HG12	1:C:154:GLU:CB	2.31	0.61
1:B:563:GLY:O	1:B:571:ASP:N	2.34	0.60
1:A:728:MET:N	1:A:771:GLN:OE1	2.33	0.60
1:B:700:ASN:ND2	1:C:784:GLN:OE1	2.34	0.60
1:A:383:LYS:HB3	1:B:979:SER:O	2.01	0.60
1:B:293:LEU:HD11	1:B:599:THR:HG22	1.84	0.60
1:B:663:ILE:HD11	1:B:669:ALA:HB2	1.83	0.59
1:C:96:GLU:OE1	1:C:96:GLU:N	2.35	0.59
1:C:411:GLN:O	1:C:421:LYS:NZ	2.35	0.59
2:H:61:ALA:HA	3:L:96:HIS:CE1	2.38	0.59
2:E:61:ALA:HA	3:F:96:HIS:CE1	2.38	0.59
1:A:979:SER:O	1:C:383:LYS:HB3	2.02	0.59
2:J:61:ALA:HA	3:K:96:HIS:CE1	2.38	0.59
1:A:143:VAL:HG13	1:A:243:ILE:HD11	1.86	0.58
1:A:344:PHE:HB2	1:A:398:VAL:HG23	1.85	0.58
1:B:451:ARG:NH2	1:B:466:SER:O	2.36	0.58
1:B:1045:HIS:HA	1:B:1063:THR:HG22	1.84	0.58
1:B:96:GLU:N	1:B:96:GLU:OE1	2.37	0.58
1:B:52:GLN:O	1:B:53:ASP:OD1	2.22	0.58
1:A:716:THR:HG22	1:A:1067:ALA:HB2	1.85	0.58
1:B:143:VAL:HG13	1:B:243:ILE:HD11	1.86	0.57
1:C:143:VAL:HG13	1:C:243:ILE:HD11	1.87	0.57
1:A:384:LEU:HA	1:A:387:LEU:HD12	1.87	0.57
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.87	0.57
1:C:961:LYS:O	1:C:964:SER:OG	2.22	0.56
1:C:293:LEU:HD11	1:C:599:THR:HG22	1.87	0.56
2:J:34:MET:HB3	2:J:79:LEU:HD22	1.87	0.56
1:A:96:GLU:N	1:A:96:GLU:OE1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.87	0.56
1:B:982:ASP:O	1:B:986:ALA:N	2.29	0.56
1:C:1069:GLU:OE1	1:C:1069:GLU:N	2.33	0.56
1:A:977:ILE:HG23	1:A:981:LEU:HD12	1.88	0.55
1:B:317:VAL:O	1:B:318:GLN:HB2	2.06	0.55
3:L:22:CYS:HB3	3:L:70:VAL:HG13	1.88	0.55
1:A:336:GLY:O	1:A:340:ASN:HB2	2.07	0.55
1:C:735:CYS:SG	1:C:736:THR:N	2.80	0.55
3:F:22:CYS:HB3	3:F:70:VAL:HG13	1.88	0.55
1:A:663:ILE:HD11	1:A:669:ALA:HB2	1.89	0.55
1:A:1111:ILE:O	1:A:1116:ASN:ND2	2.40	0.55
1:A:641:GLN:NE2	1:A:645:GLY:O	2.40	0.54
1:C:560:GLN:O	1:C:574:ARG:NH2	2.30	0.54
1:B:1113:THR:HG22	1:B:1135:TYR:HB3	1.88	0.54
1:A:614:CYS:N	1:A:641:GLN:OE1	2.41	0.54
3:K:22:CYS:HB3	3:K:70:VAL:HG13	1.88	0.54
1:A:247:THR:O	2:H:102:SER:HB2	2.08	0.54
1:A:1123:CYS:SG	1:A:1129:ILE:HD13	2.48	0.54
1:A:148:ASN:OD1	3:L:50:ASN:HB2	2.08	0.54
1:B:247:THR:O	2:E:102:SER:HB2	2.08	0.53
3:L:27:ILE:HD13	3:L:70:VAL:HG11	1.90	0.53
3:F:27:ILE:HD13	3:F:70:VAL:HG11	1.90	0.53
1:C:52:GLN:O	1:C:53:ASP:OD1	2.27	0.53
1:C:286:VAL:HG23	1:C:303:PHE:CE2	2.44	0.53
1:C:575:ASP:OD2	1:C:578:THR:OG1	2.27	0.53
3:K:27:ILE:HD13	3:K:70:VAL:HG11	1.90	0.53
1:C:733:VAL:HG11	1:C:1001:LEU:HD21	1.91	0.52
1:C:247:THR:O	2:J:102:SER:HB2	2.09	0.52
1:C:390:THR:O	1:C:520:THR:OG1	2.26	0.52
1:C:415:ILE:HD13	1:C:419:ASN:HD22	1.74	0.52
1:A:99:ASN:OD1	1:A:190:ARG:NH2	2.43	0.52
2:H:61:ALA:HA	3:L:96:HIS:HE1	1.74	0.52
1:B:99:ASN:OD1	1:B:190:ARG:NH2	2.43	0.52
1:C:736:THR:O	1:C:740:CYS:N	2.32	0.52
1:C:816:GLU:OE2	1:C:1052:SER:N	2.37	0.51
1:B:653:VAL:HG12	1:B:655:ASN:H	1.76	0.51
1:B:311:GLN:NE2	1:B:313:SER:O	2.44	0.51
1:B:524:PRO:O	1:B:525:LYS:C	2.49	0.51
1:A:228:ASP:OD1	1:A:228:ASP:N	2.43	0.51
1:A:124:THR:O	1:A:175:PHE:N	2.37	0.51
1:A:380:SER:N	1:B:980:ARG:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASN:OD1	1:A:414:ASN:N	2.44	0.50
1:C:527:SER:OG	1:C:577:GLN:NE2	2.42	0.50
2:E:61:ALA:HA	3:F:96:HIS:HE1	1.74	0.50
2:J:61:ALA:HA	3:K:96:HIS:HE1	1.75	0.50
1:C:898:GLN:O	1:C:902:ARG:HG2	2.11	0.50
1:C:124:THR:O	1:C:175:PHE:N	2.34	0.50
1:A:378:GLY:CA	1:B:970:ILE:HG21	2.38	0.50
1:A:1069:GLU:OE1	1:A:1069:GLU:N	2.37	0.50
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.94	0.50
1:A:293:LEU:HD11	1:A:599:THR:HG22	1.94	0.49
1:C:187:LYS:NZ	1:C:213:VAL:O	2.45	0.49
1:C:557:LEU:O	1:C:574:ARG:NH2	2.45	0.49
1:B:124:THR:O	1:B:175:PHE:N	2.36	0.49
3:F:46:VAL:HA	3:F:57:ILE:HG13	1.94	0.49
1:A:922:ASN:O	1:A:926:SER:OG	2.27	0.49
1:B:29:THR:HG22	1:B:30:ASN:H	1.77	0.49
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.94	0.49
1:C:347:VAL:HG22	1:C:419:ASN:HB3	1.95	0.49
3:K:46:VAL:HA	3:K:57:ILE:HG13	1.94	0.49
1:B:593:SER:OG	1:B:610:GLN:OE1	2.32	0.48
1:B:567:ALA:CB	1:C:960:VAL:HG11	2.42	0.48
1:A:733:VAL:HG11	1:A:1001:LEU:HD21	1.96	0.48
1:B:595:ILE:HG23	1:B:661:ILE:HG21	1.94	0.48
1:C:613:ASN:OD1	1:C:614:CYS:N	2.46	0.48
1:A:216:LEU:HD12	1:A:217:PRO:HD2	1.95	0.48
1:B:723:ILE:HD13	1:B:942:LEU:HD13	1.94	0.48
1:C:726:VAL:HG23	1:C:1056:GLY:HA2	1.95	0.48
1:B:293:LEU:HD11	1:B:599:THR:CG2	2.43	0.48
1:A:376:CYS:HB3	1:A:379:VAL:HG13	1.95	0.48
1:B:286:VAL:HG23	1:B:303:PHE:CE2	2.49	0.48
1:C:388:CYS:HB3	1:C:519:ALA:HB1	1.94	0.48
1:A:342:THR:O	1:A:506:ARG:NH2	2.45	0.47
1:A:711:ILE:HD12	1:A:1093:VAL:HG11	1.95	0.47
1:C:100:ILE:HA	1:C:243:ILE:HG22	1.97	0.47
3:L:46:VAL:HA	3:L:57:ILE:HG13	1.95	0.47
1:B:148:ASN:OD1	3:F:50:ASN:HB2	2.13	0.47
1:A:898:GLN:O	1:A:902:ARG:HG2	2.14	0.47
1:C:228:ASP:OD1	1:C:228:ASP:N	2.47	0.47
1:B:562:PHE:O	1:C:43:PHE:N	2.32	0.47
1:B:1128:GLY:HA2	5:B:1307:NAG:H81	1.97	0.47
1:C:148:ASN:OD1	3:K:50:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1073:THR:O	1:A:1094:SER:N	2.48	0.47
1:C:721:THR:HG23	1:C:1058:VAL:HG13	1.95	0.47
1:A:187:LYS:NZ	1:A:213:VAL:O	2.48	0.47
1:B:802:ILE:HD12	1:B:875:LEU:HD21	1.97	0.47
1:C:900:ALA:HB1	1:C:910:GLN:HB2	1.97	0.47
1:A:823:VAL:HG23	1:A:942:LEU:HD12	1.97	0.46
1:B:187:LYS:NZ	1:B:213:VAL:O	2.48	0.46
1:A:337:GLU:OE2	1:A:353:LYS:NZ	2.47	0.46
1:A:578:THR:O	1:A:580:GLU:N	2.48	0.46
2:H:99:SER:HB3	2:H:113:LEU:HD23	1.97	0.46
1:A:29:THR:HG22	1:A:30:ASN:H	1.78	0.46
1:B:976:ASP:O	1:B:980:ARG:HG3	2.16	0.46
1:C:578:THR:O	1:C:580:GLU:N	2.46	0.46
2:J:99:SER:HB3	2:J:113:LEU:HD23	1.97	0.46
1:A:388:CYS:HB3	1:A:519:ALA:HB1	1.97	0.46
1:B:143:VAL:HA	1:B:154:GLU:HA	1.98	0.46
1:A:712:PRO:HA	1:A:1069:GLU:HA	1.98	0.46
2:E:99:SER:HB3	2:E:113:LEU:HD23	1.97	0.46
1:A:1122:ASN:ND2	1:A:1124:ASP:OD2	2.49	0.45
1:C:29:THR:HG22	1:C:30:ASN:H	1.80	0.45
1:A:390:THR:O	1:A:520:THR:OG1	2.34	0.45
1:A:877:GLY:O	1:A:881:SER:OG	2.27	0.45
1:C:1078:ILE:HD12	1:C:1112:ILE:HD13	1.98	0.45
1:A:733:VAL:O	1:A:761:ASN:ND2	2.48	0.45
1:B:1008:GLN:OE1	1:B:1011:ARG:NH1	2.50	0.45
1:B:454:ARG:NH1	1:B:456:SER:OG	2.49	0.45
1:B:329:ILE:HG21	1:B:332:LEU:CD2	2.46	0.45
1:C:373:THR:HB	1:C:432:ALA:HB3	1.98	0.45
1:A:100:ILE:HA	1:A:243:ILE:HG22	1.99	0.45
1:A:575:ASP:HB3	1:A:578:THR:O	2.16	0.45
1:C:1045:HIS:HA	1:C:1063:THR:HG22	1.97	0.45
1:B:733:VAL:HG11	1:B:1001:LEU:HD21	1.99	0.45
1:B:1127:ILE:HD12	1:C:917:GLN:OE1	2.17	0.45
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.24	0.45
1:A:875:LEU:HD11	1:A:1049:PHE:HB3	1.99	0.45
1:B:398:VAL:HG22	1:B:506:ARG:HG2	1.98	0.45
1:B:721:THR:HG23	1:B:1058:VAL:HG13	1.99	0.45
1:C:193:VAL:HG23	1:C:223:LEU:HD22	1.98	0.45
1:C:53:ASP:HB2	1:C:55:PHE:CE2	2.51	0.45
3:F:45:LEU:HD21	3:F:48:TYR:HB3	1.99	0.44
1:A:913:LEU:C	1:A:913:LEU:HD13	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:VAL:HA	1:C:154:GLU:HA	2.00	0.44
1:A:574:ARG:HE	1:A:579:LEU:HB3	1.83	0.44
1:C:31:SER:OG	1:C:60:SER:N	2.46	0.44
3:K:45:LEU:HD21	3:K:48:TYR:HB3	1.99	0.44
1:A:143:VAL:HA	1:A:154:GLU:HA	1.99	0.44
1:B:1104:ARG:CZ	1:C:901:TYR:CE1	3.00	0.44
1:B:422:LEU:HD21	1:B:509:VAL:HG11	1.99	0.44
1:B:700:ASN:O	1:C:786:TYR:HA	2.18	0.44
1:A:1104:ARG:HD2	1:B:901:TYR:CZ	2.53	0.44
1:B:228:ASP:OD1	1:B:228:ASP:N	2.49	0.44
1:B:347:VAL:HG22	1:B:419:ASN:HB3	2.00	0.43
1:C:414:ASN:OD1	1:C:414:ASN:N	2.50	0.43
1:C:718:SER:OG	1:C:1063:THR:OG1	2.36	0.43
1:C:1004:TYR:CE2	1:C:1008:GLN:HG3	2.53	0.43
1:C:338:VAL:HG11	1:C:394:ALA:HB1	1.99	0.43
3:L:53:ARG:NH2	3:L:59:GLU:HG2	2.34	0.43
1:A:808:LYS:NZ	1:A:817:ASP:OD2	2.30	0.43
1:B:100:ILE:HA	1:B:243:ILE:HG22	1.99	0.43
3:L:45:LEU:HD21	3:L:48:TYR:HB3	1.99	0.43
1:C:1138:LEU:HD11	1:C:1142:LEU:HD13	2.00	0.43
2:H:34:MET:HG2	2:H:72:ARG:NH2	2.34	0.43
1:A:965:SER:HB2	1:A:967:PHE:CE2	2.54	0.43
1:A:1028:GLU:OE1	1:A:1036:ARG:NH1	2.50	0.43
1:B:913:LEU:HD13	1:B:913:LEU:C	2.39	0.43
2:E:34:MET:HG2	2:E:72:ARG:NH2	2.34	0.43
1:A:57:PRO:O	1:A:60:SER:OG	2.22	0.43
1:B:27:ALA:HB3	1:B:64:TRP:NE1	2.34	0.43
1:B:288:CYS:O	1:B:295:GLU:HG3	2.19	0.43
1:C:716:THR:HG23	1:C:1065:VAL:HB	2.01	0.43
1:A:1042:LYS:NZ	1:B:887:ALA:O	2.51	0.42
1:B:711:ILE:HD12	1:B:1093:VAL:HG11	2.01	0.42
1:C:27:ALA:HB3	1:C:64:TRP:NE1	2.34	0.42
1:C:974:LEU:HD11	1:C:990:ILE:HG12	2.01	0.42
3:F:53:ARG:NH2	3:F:59:GLU:HG2	2.34	0.42
2:J:34:MET:HG2	2:J:72:ARG:NH2	2.34	0.42
3:K:53:ARG:NH2	3:K:59:GLU:HG2	2.34	0.42
1:B:319:PRO:HA	1:B:535:CYS:SG	2.58	0.42
1:A:148:ASN:ND2	3:L:51:SER:OG	2.47	0.42
1:B:361:ASP:HA	1:B:524:PRO:HG3	2.00	0.42
1:C:194:PHE:HB3	1:C:201:PHE:CZ	2.54	0.42
1:A:27:ALA:HB3	1:A:64:TRP:NE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:LEU:N	1:A:560:GLN:OE1	2.40	0.42
1:B:578:THR:O	1:B:580:GLU:N	2.47	0.42
1:B:753:TYR:HB3	1:B:756:PHE:CD2	2.54	0.42
1:B:131:CYS:HA	1:B:166:CYS:HA	2.02	0.42
1:B:600:ASN:OD1	1:B:600:ASN:O	2.37	0.42
1:B:723:ILE:HG22	1:B:945:LEU:HD13	2.01	0.42
1:A:193:VAL:HG23	1:A:223:LEU:HD22	2.01	0.42
1:B:724:LEU:HD11	1:B:1025:LYS:HD2	2.02	0.42
1:A:13:SER:OG	1:A:14:GLN:N	2.53	0.42
1:A:96:GLU:HB3	1:A:260:ALA:CB	2.50	0.42
1:A:293:LEU:O	1:A:296:THR:OG1	2.30	0.42
1:A:595:ILE:HG23	1:A:661:ILE:HG21	2.01	0.42
1:A:726:VAL:HG23	1:A:1056:GLY:HA2	2.02	0.42
1:A:900:ALA:HB1	1:A:910:GLN:HB2	2.02	0.42
1:B:194:PHE:HB3	1:B:201:PHE:CZ	2.55	0.42
1:A:906:ILE:HD13	1:A:1046:LEU:HD21	2.01	0.42
1:B:712:PRO:HA	1:B:1069:GLU:HA	2.02	0.42
1:C:305:VAL:HB	1:C:599:THR:HG23	2.02	0.42
3:L:32:VAL:HG21	3:L:70:VAL:HG21	2.02	0.42
1:A:122:ASN:OD1	1:A:125:ASN:O	2.38	0.41
1:B:1104:ARG:NH2	1:C:901:TYR:CE1	2.87	0.41
1:B:390:THR:HG22	1:B:517:ALA:O	2.20	0.41
1:C:598:GLY:O	1:C:601:THR:N	2.52	0.41
1:B:575:ASP:HB3	1:B:578:THR:O	2.21	0.41
1:B:1127:ILE:HD12	1:C:917:GLN:CD	2.41	0.41
2:H:102:SER:OG	2:H:103:GLY:N	2.54	0.41
3:K:32:VAL:HG21	3:K:70:VAL:HG21	2.03	0.41
1:A:388:CYS:HB3	1:A:519:ALA:CB	2.51	0.41
1:A:1004:TYR:CZ	1:A:1008:GLN:HG3	2.55	0.41
2:H:98:ARG:HG2	2:H:115:VAL:HB	2.02	0.41
1:A:784:GLN:OE1	1:C:700:ASN:ND2	2.54	0.41
1:B:564:ARG:NH2	1:C:42:VAL:HG21	2.36	0.41
3:F:32:VAL:HG21	3:F:70:VAL:HG21	2.03	0.41
1:A:1113:THR:HG22	1:A:1135:TYR:HB3	2.03	0.41
3:K:4:LEU:HD23	3:K:4:LEU:HA	1.86	0.41
1:A:194:PHE:HB3	1:A:201:PHE:CZ	2.56	0.41
1:B:96:GLU:HB3	1:B:260:ALA:CB	2.51	0.41
1:C:13:SER:OG	1:C:14:GLN:N	2.54	0.41
1:C:148:ASN:ND2	3:K:51:SER:OG	2.49	0.41
1:C:711:ILE:HD12	1:C:1093:VAL:HG11	2.02	0.41
2:J:102:SER:OG	2:J:103:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ASN:O	1:B:786:TYR:HA	2.21	0.41
1:B:13:SER:OG	1:B:14:GLN:N	2.52	0.41
1:C:331:ASN:O	1:C:359:VAL:HG12	2.21	0.41
1:C:913:LEU:HD22	1:C:920:ILE:HD13	2.03	0.41
2:E:98:ARG:HG2	2:E:115:VAL:HB	2.03	0.41
2:J:98:ARG:HG2	2:J:115:VAL:HB	2.03	0.41
1:A:194:PHE:CE1	1:A:203:ILE:HG23	2.56	0.40
1:C:195:LYS:HG2	1:C:197:ILE:HG12	2.03	0.40
1:C:575:ASP:HB3	1:C:578:THR:O	2.20	0.40
1:C:712:PRO:HA	1:C:1069:GLU:HA	2.03	0.40
1:A:297:LYS:HE3	1:A:599:THR:HG21	2.02	0.40
1:A:767:ILE:O	1:A:770:GLU:HG2	2.21	0.40
1:C:48:LEU:CD1	1:C:302:SER:HA	2.51	0.40
1:C:1073:THR:HB	1:C:1094:SER:HB3	2.03	0.40
1:A:802:ILE:HD12	1:A:875:LEU:HD21	2.03	0.40
1:A:746:CYS:HB2	1:A:974:LEU:HD21	2.03	0.40
1:C:913:LEU:HD13	1:C:913:LEU:C	2.41	0.40
2:E:83:MET:HB3	2:E:86:LEU:HD21	2.03	0.40
3:F:38:LYS:HG2	3:F:83:ALA:HB2	2.04	0.40
3:K:38:LYS:HG2	3:K:83:ALA:HB2	2.04	0.40
1:A:1139:GLN:N	1:A:1140:PRO:HD2	2.37	0.40
1:B:148:ASN:ND2	3:F:51:SER:OG	2.48	0.40
1:C:96:GLU:HB3	1:C:260:ALA:CB	2.51	0.40
1:C:122:ASN:OD1	1:C:125:ASN:O	2.38	0.40
2:E:62:ASP:H	3:F:96:HIS:HE1	1.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1048/1285 (82%)	1013 (97%)	35 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1044/1285 (81%)	1009 (97%)	34 (3%)	1 (0%)	48	83
1	C	1045/1285 (81%)	1003 (96%)	42 (4%)	0	100	100
2	E	124/231 (54%)	120 (97%)	4 (3%)	0	100	100
2	H	124/231 (54%)	120 (97%)	4 (3%)	0	100	100
2	J	124/231 (54%)	120 (97%)	4 (3%)	0	100	100
3	F	106/214 (50%)	103 (97%)	3 (3%)	0	100	100
3	K	106/214 (50%)	103 (97%)	3 (3%)	0	100	100
3	L	106/214 (50%)	103 (97%)	3 (3%)	0	100	100
All	All	3827/5190 (74%)	3694 (96%)	132 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	318	GLN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	927/1109 (84%)	920 (99%)	7 (1%)	79	85
1	B	924/1109 (83%)	911 (99%)	13 (1%)	62	76
1	C	925/1109 (83%)	917 (99%)	8 (1%)	75	83
2	E	102/193 (53%)	102 (100%)	0	100	100
2	H	102/193 (53%)	102 (100%)	0	100	100
2	J	102/193 (53%)	102 (100%)	0	100	100
3	F	91/183 (50%)	90 (99%)	1 (1%)	70	80
3	K	91/183 (50%)	90 (99%)	1 (1%)	70	80
3	L	91/183 (50%)	90 (99%)	1 (1%)	70	80
All	All	3355/4455 (75%)	3324 (99%)	31 (1%)	74	83

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	A	65	PHE
1	A	104	TRP
1	A	374	PHE
1	A	716	THR
1	A	875	LEU
1	A	926	SER
1	B	29	THR
1	B	44	ARG
1	B	65	PHE
1	B	104	TRP
1	B	307	LYS
1	B	318	GLN
1	B	329	ILE
1	B	340	ASN
1	B	374	PHE
1	B	391	ASN
1	B	788	THR
1	B	875	LEU
1	B	1069	GLU
1	C	29	THR
1	C	44	ARG
1	C	65	PHE
1	C	104	TRP
1	C	374	PHE
1	C	612	VAL
1	C	716	THR
1	C	875	LEU
3	L	25	ASN
3	F	25	ASN
3	K	25	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	82	GLN
3	L	96	HIS
2	E	82	GLN
3	F	96	HIS
2	J	82	GLN
3	K	96	HIS



### 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	$\# Z  > 2$
4	NAG	D	1	4,1	14,14,15	0.24	0	17,19,21	0.34	0
4	NAG	D	2	4	14,14,15	0.18	0	17,19,21	0.38	0
4	NAG	G	1	4,1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	G	2	4	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	I	1	4,1	14,14,15	0.20	0	17,19,21	0.49	0
4	NAG	I	2	4	14,14,15	0.21	0	17,19,21	0.39	0
4	NAG	M	1	4,1	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	M	2	4	14,14,15	0.22	0	17,19,21	0.38	0
4	NAG	N	1	4,1	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	N	2	4	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	O	1	4,1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	O	2	4	14,14,15	0.22	0	17,19,21	0.38	0
4	NAG	P	1	4,1	14,14,15	0.18	0	17,19,21	0.48	0
4	NAG	P	2	4	14,14,15	0.21	0	17,19,21	0.38	0
4	NAG	Q	1	4,1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	Q	2	4	14,14,15	0.29	0	17,19,21	0.41	0
4	NAG	R	1	4,1	14,14,15	0.25	0	17,19,21	0.34	0
4	NAG	R	2	4	14,14,15	0.17	0	17,19,21	0.43	0
4	NAG	S	1	4,1	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	S	2	4	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	T	1	4,1	14,14,15	0.44	0	17,19,21	0.66	1 (5%)
4	NAG	T	2	4	14,14,15	0.23	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	U	1	4,1	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	U	2	4	14,14,15	0.21	0	17,19,21	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	0/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	1	NAG	C1-O5-C5	2.17	115.13	112.19

There are no chirality outliers.

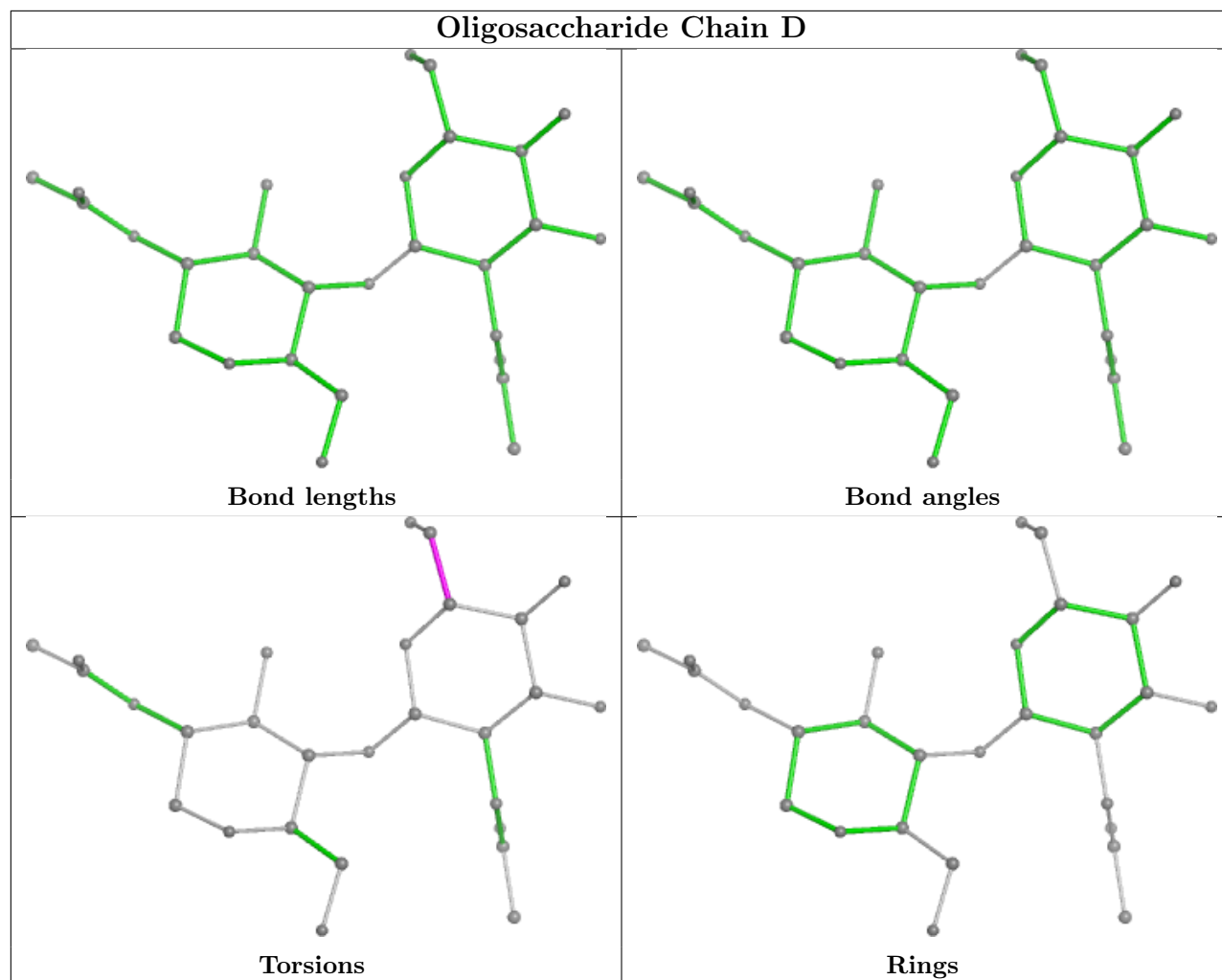
All (30) torsion outliers are listed below:

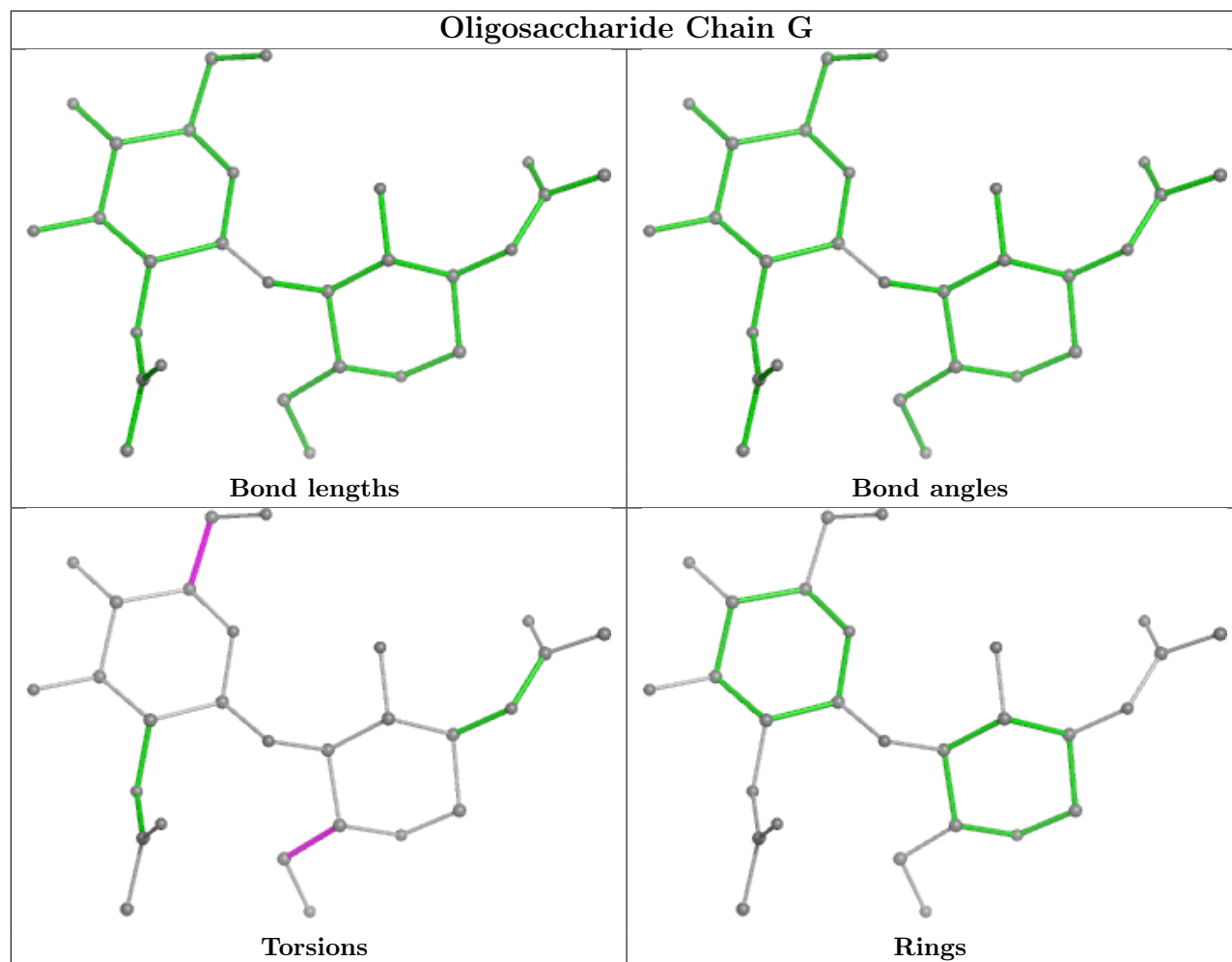
Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6

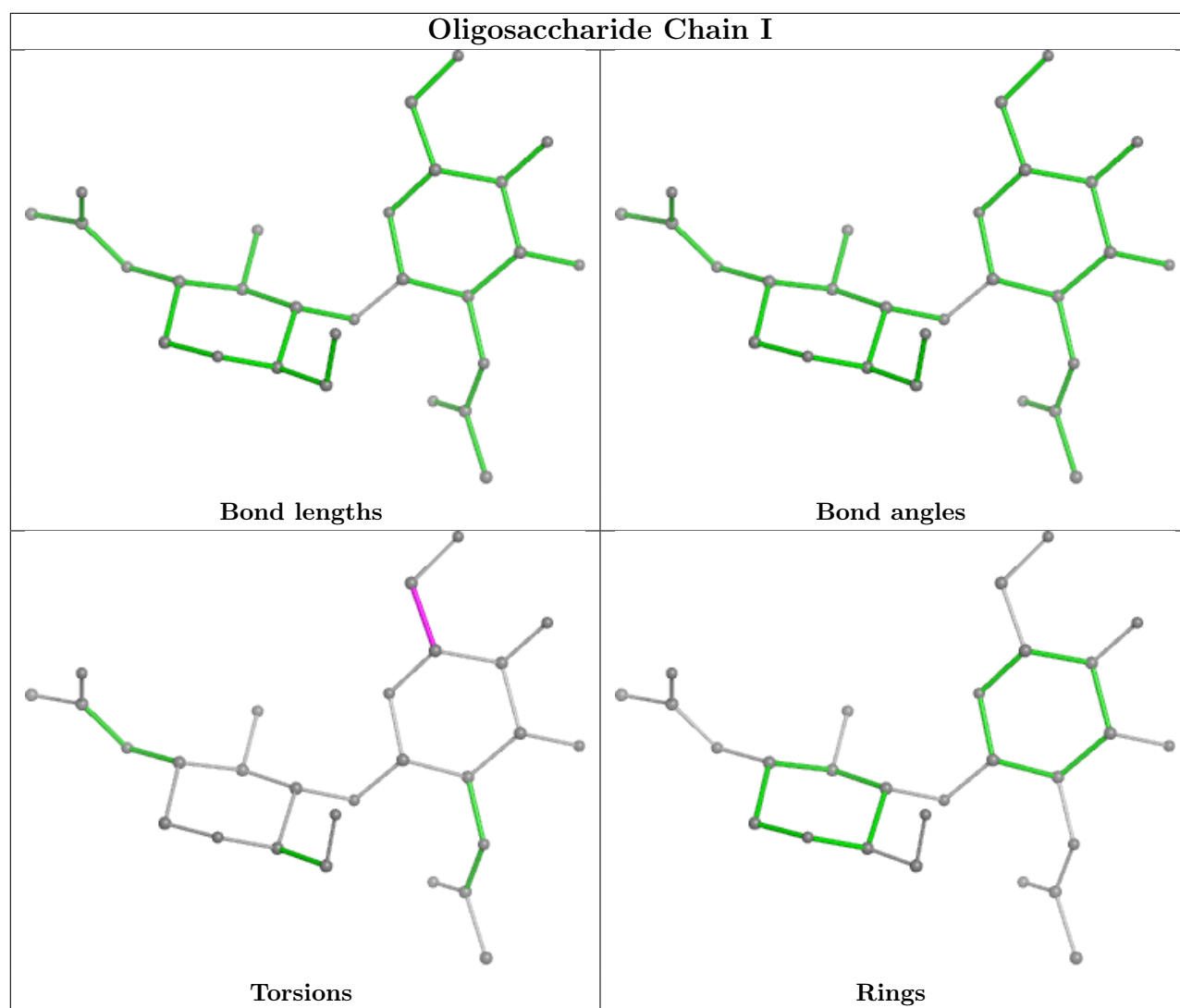
There are no ring outliers.

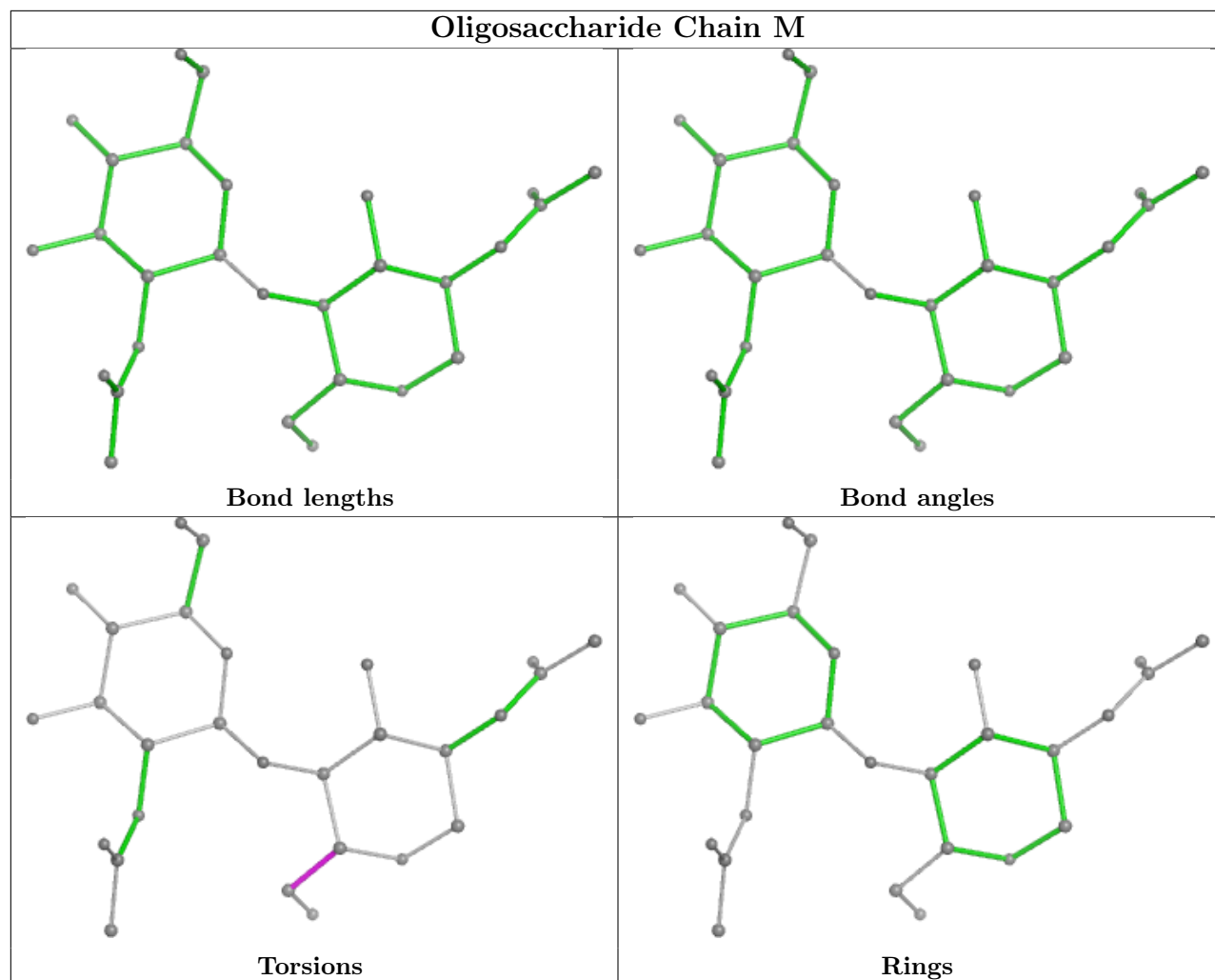
No monomer is involved in short contacts.

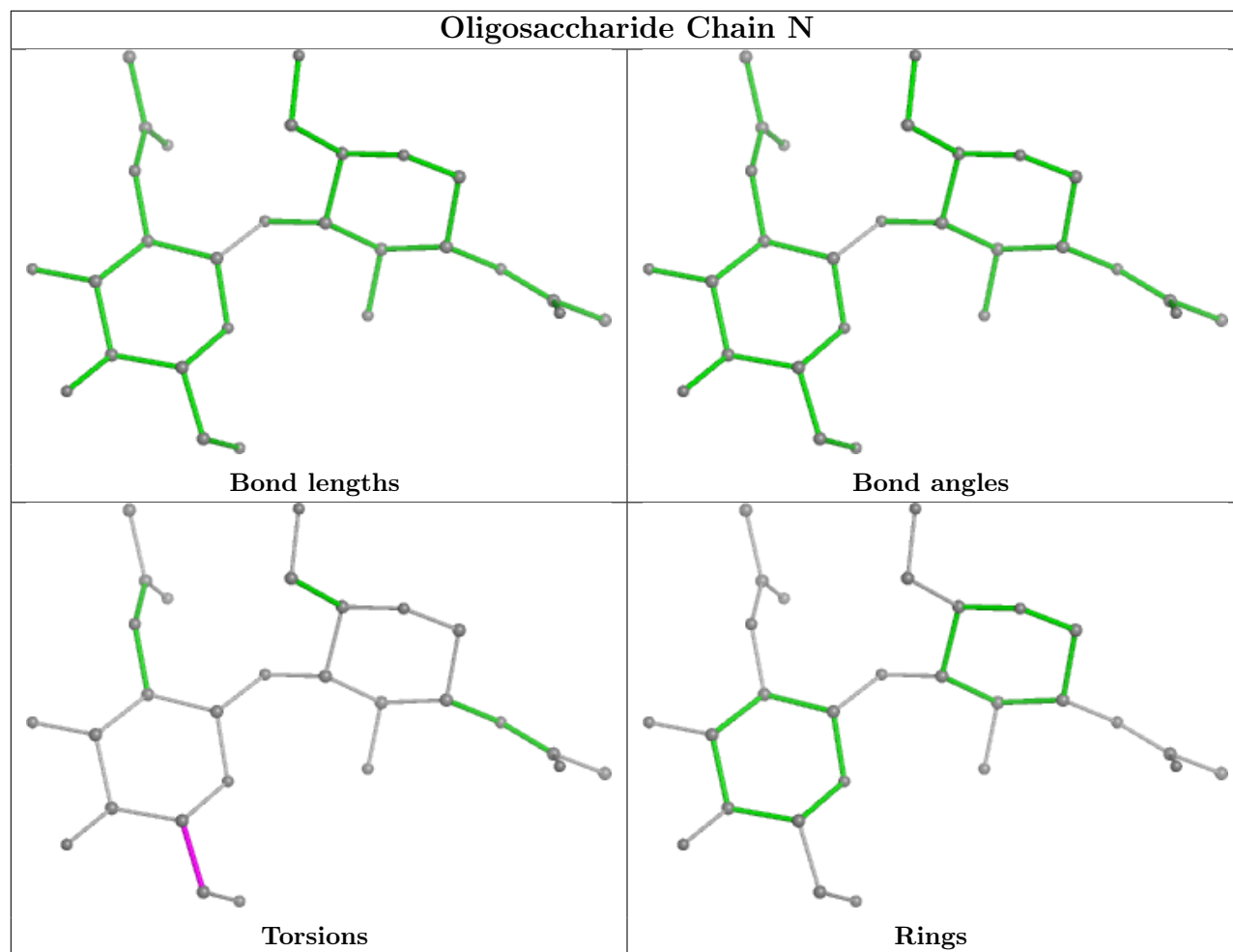
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



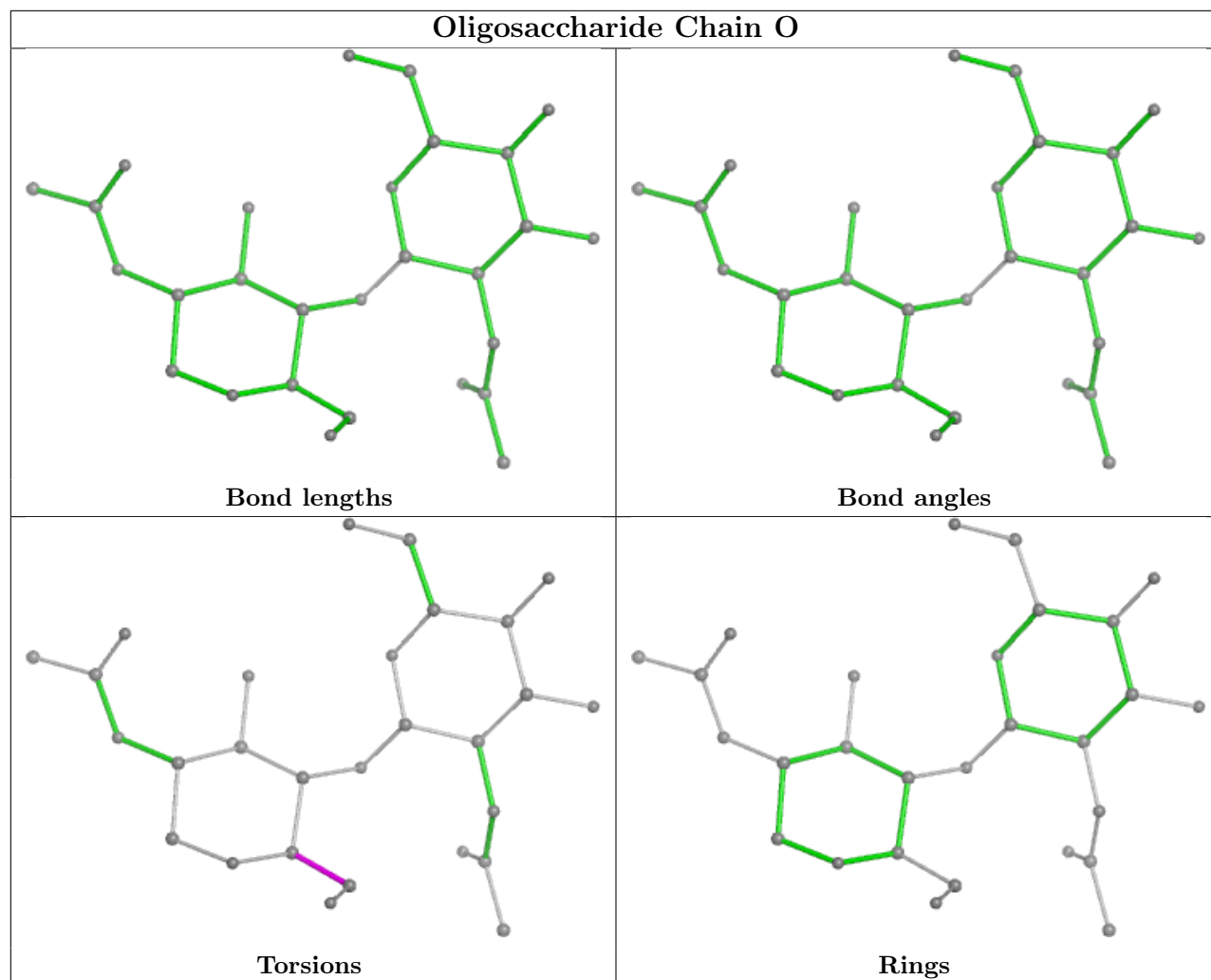


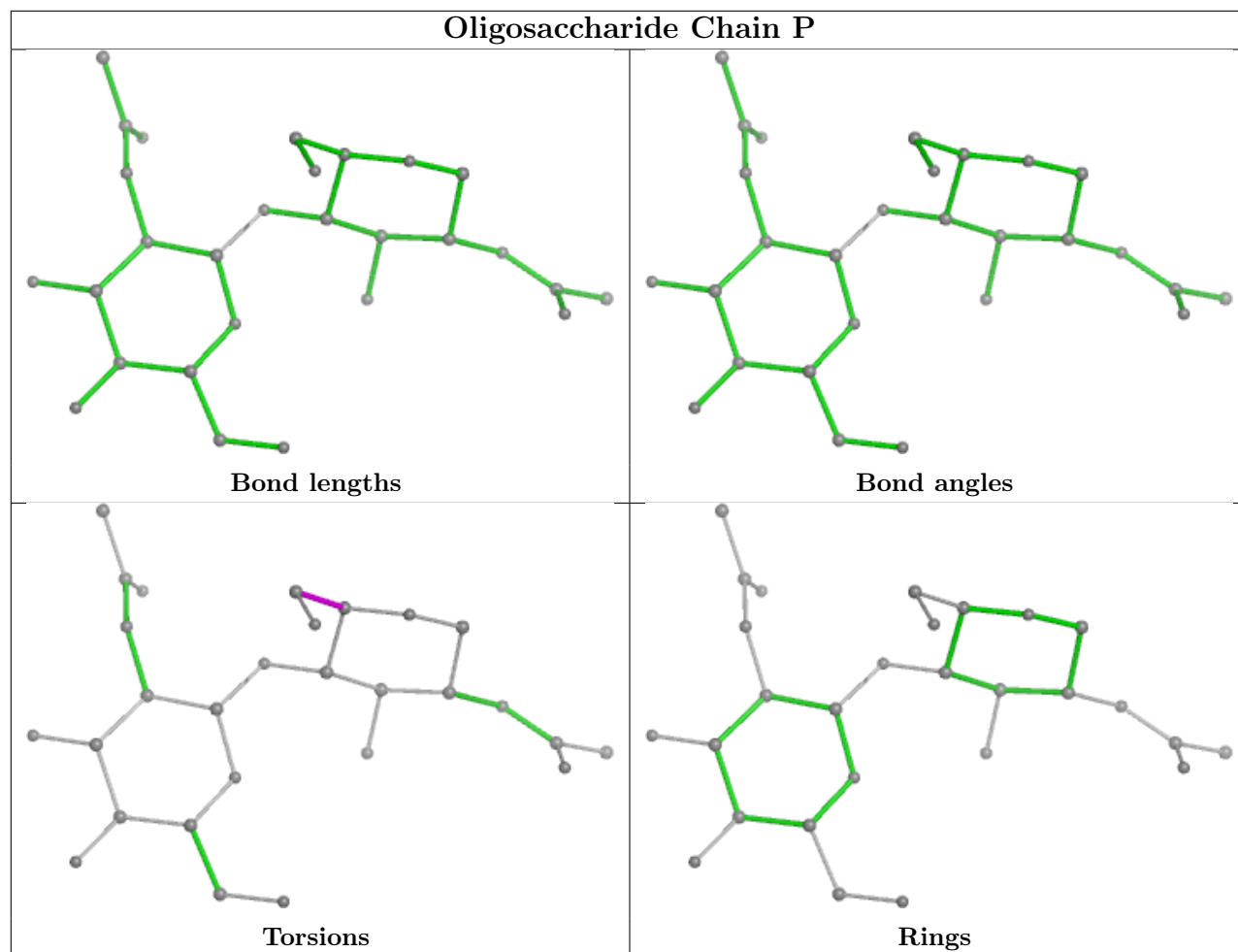


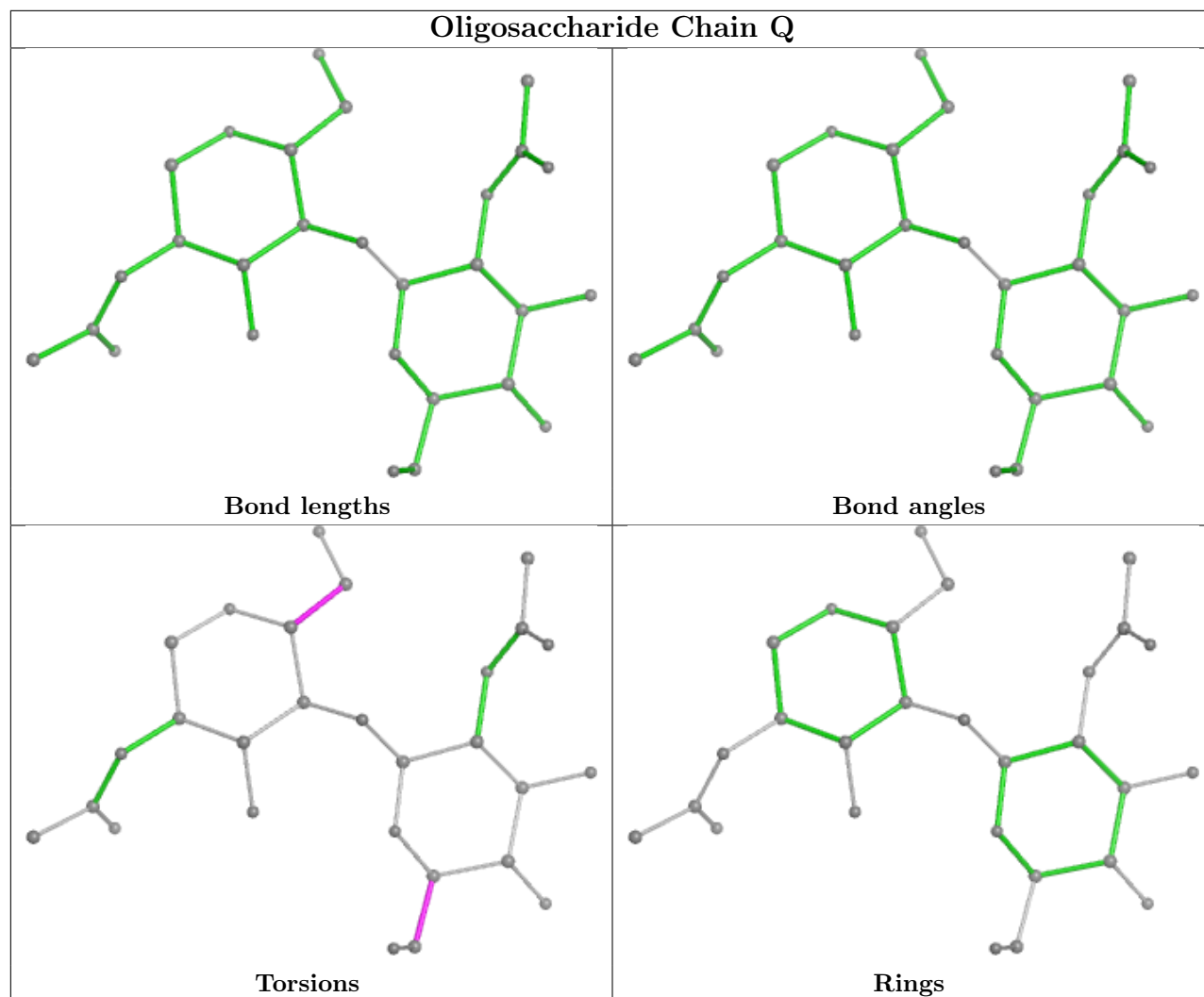


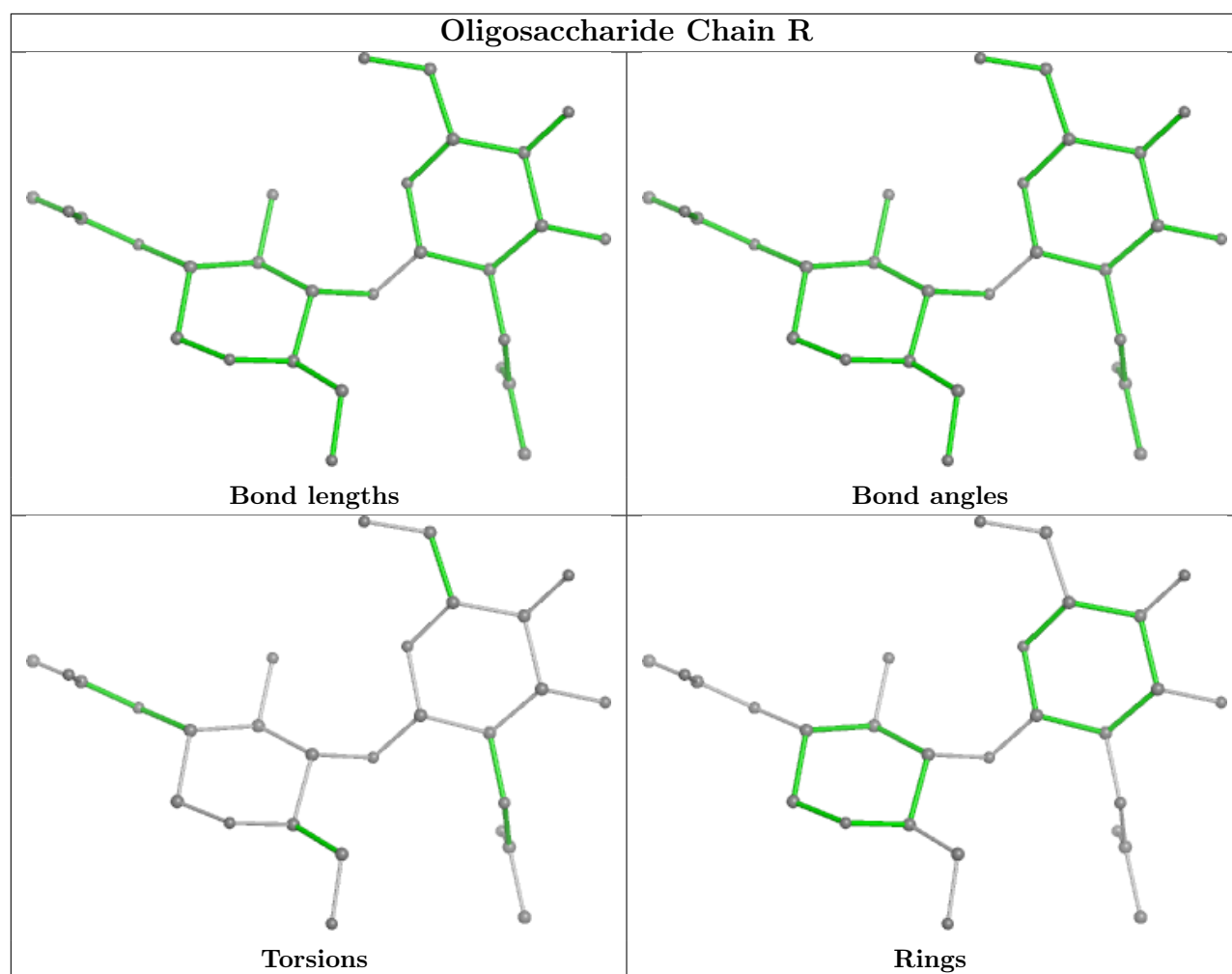


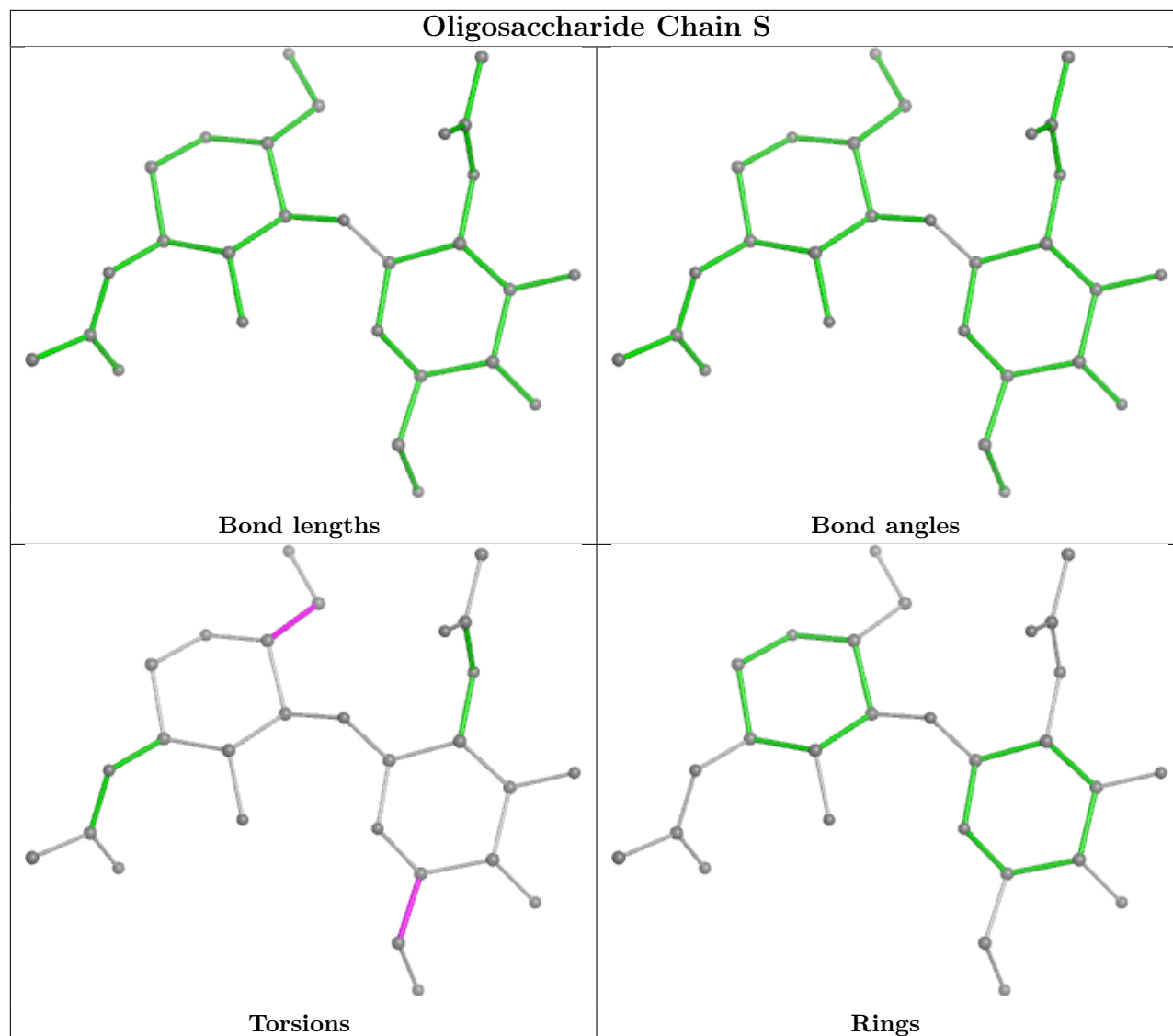


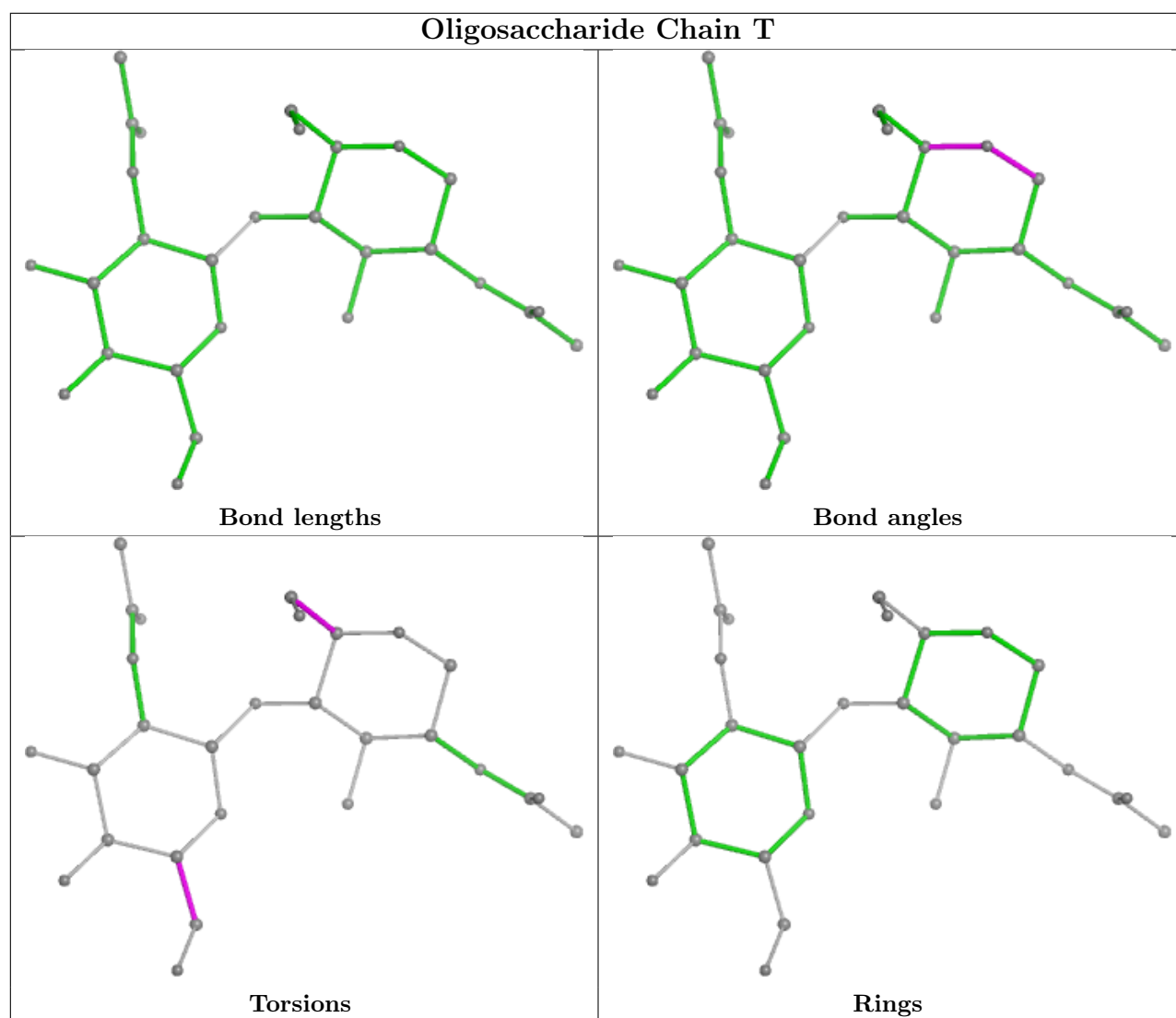


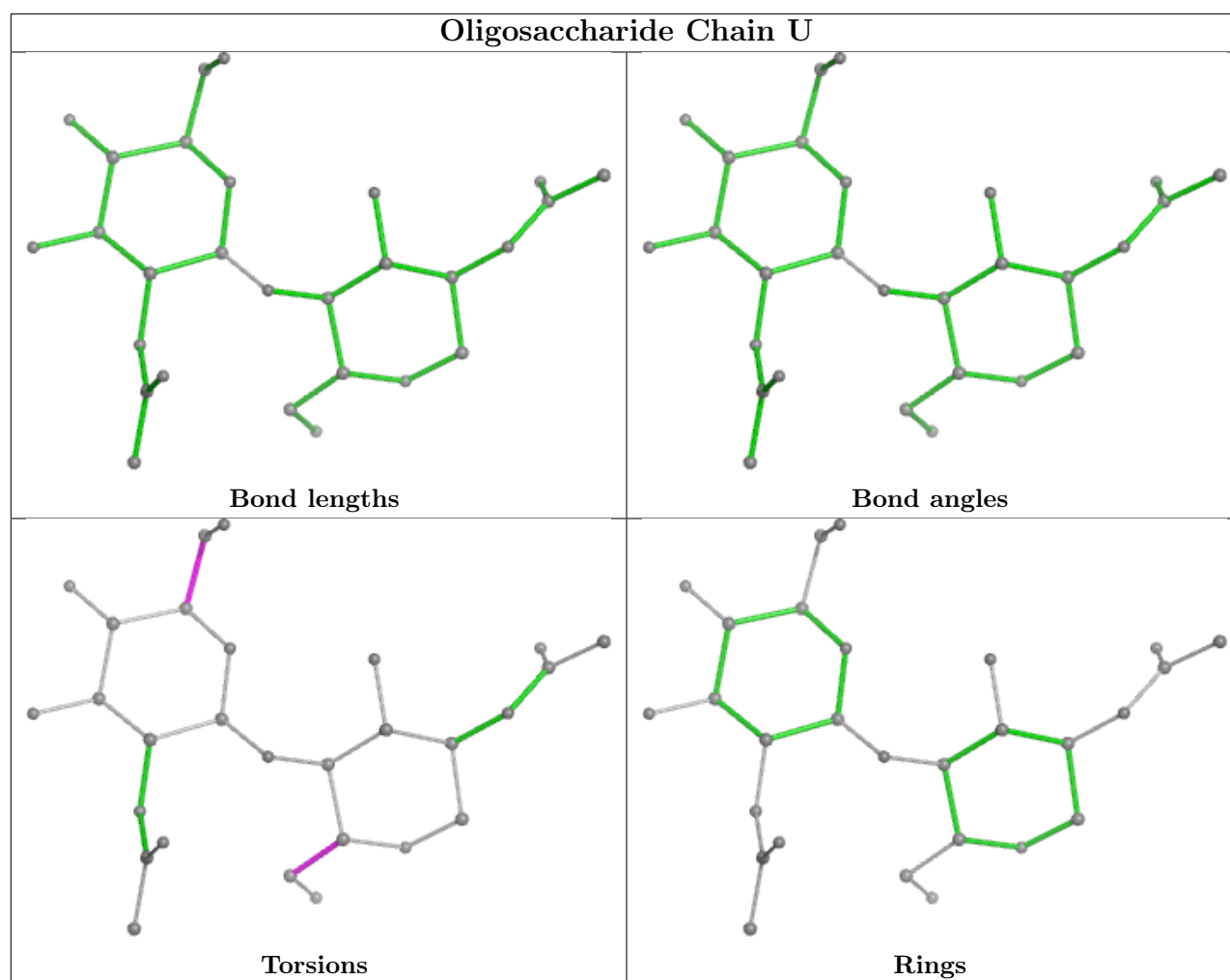












## 5.6 Ligand geometry [i](#)

29 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	$\# Z  > 2$
5	NAG	A	1307	1	14,14,15	0.19	0	17,19,21	0.35	0
5	NAG	B	1302	1	14,14,15	0.28	0	17,19,21	0.43	0
5	NAG	B	1306	1	14,14,15	0.28	0	17,19,21	0.44	0
5	NAG	C	1309	1	14,14,15	0.25	0	17,19,21	0.47	0
5	NAG	B	1304	1	14,14,15	0.57	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	1310	1	14,14,15	0.21	0	17,19,21	0.53	0
5	NAG	A	1303	1	14,14,15	0.19	0	17,19,21	0.38	0
5	NAG	B	1307	1	14,14,15	0.26	0	17,19,21	0.40	0
5	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.48	0
5	NAG	C	1302	1	14,14,15	0.17	0	17,19,21	0.38	0
5	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.36	0
5	NAG	A	1308	1	14,14,15	0.48	0	17,19,21	0.85	1 (5%)
5	NAG	A	1302	1	14,14,15	0.30	0	17,19,21	0.71	1 (5%)
5	NAG	C	1304	1	14,14,15	0.20	0	17,19,21	0.49	0
5	NAG	C	1301	1	14,14,15	0.24	0	17,19,21	0.62	0
5	NAG	A	1306	1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	B	1309	1	14,14,15	0.17	0	17,19,21	0.35	0
5	NAG	A	1301	1	14,14,15	0.41	0	17,19,21	0.74	1 (5%)
5	NAG	C	1305	1	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	A	1304	1	14,14,15	0.18	0	17,19,21	0.37	0
5	NAG	C	1303	1	14,14,15	0.21	0	17,19,21	0.37	0
5	NAG	B	1308	1	14,14,15	0.34	0	17,19,21	0.51	0
5	NAG	B	1303	1	14,14,15	0.26	0	17,19,21	0.62	1 (5%)
5	NAG	B	1301	1	14,14,15	0.26	0	17,19,21	0.53	0
5	NAG	A	1310	1	14,14,15	0.48	0	17,19,21	1.05	1 (5%)
5	NAG	C	1307	1	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	C	1306	1	14,14,15	0.26	0	17,19,21	0.33	0
5	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	C	1308	1	14,14,15	0.39	0	17,19,21	0.63	1 (5%)

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

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

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1310	NAG	C1-O5-C5	3.86	117.42	112.19
5	A	1308	NAG	C1-O5-C5	3.11	116.41	112.19
5	A	1301	NAG	C1-O5-C5	2.53	115.61	112.19
5	B	1303	NAG	C1-O5-C5	2.16	115.11	112.19
5	A	1302	NAG	C1-O5-C5	2.13	115.08	112.19
5	C	1308	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1301	NAG	O5-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
5	B	1305	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	B	1309	NAG	C4-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	C	1307	NAG	O5-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	B	1305	NAG	C4-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	A	1309	NAG	C4-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	B	1306	NAG	O5-C5-C6-O6
5	B	1303	NAG	C4-C5-C6-O6
5	C	1307	NAG	C4-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	A	1309	NAG	C1-C2-N2-C7
5	C	1302	NAG	C4-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	C	1304	NAG	C1-C2-N2-C7
5	B	1307	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1307	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

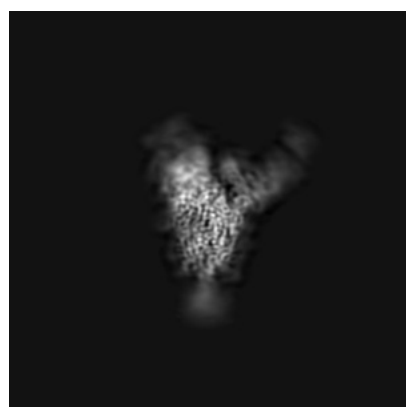
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13870. These allow visual inspection of the internal detail of the map and identification of artifacts.

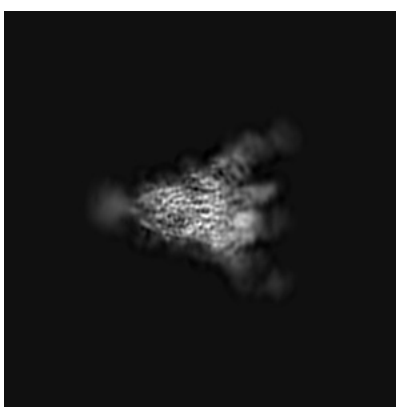
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

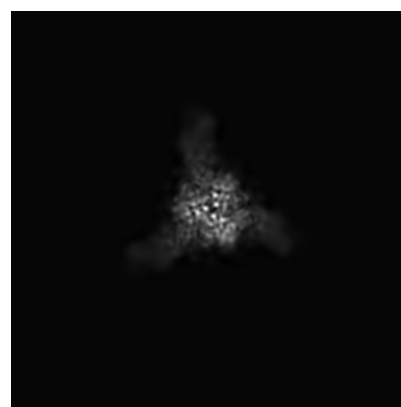
#### 6.1.1 Primary map



X



Y



Z

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

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

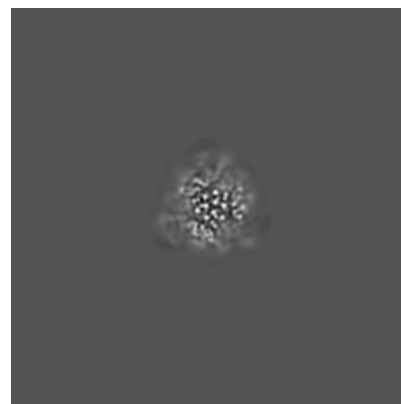
#### 6.2.1 Primary map



X Index: 140



Y Index: 140

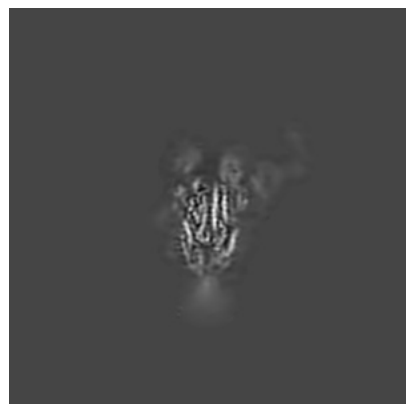


Z Index: 140

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

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

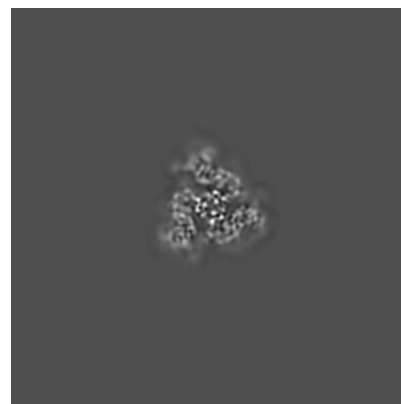
### 6.3.1 Primary map



X Index: 143



Y Index: 144



Z Index: 147

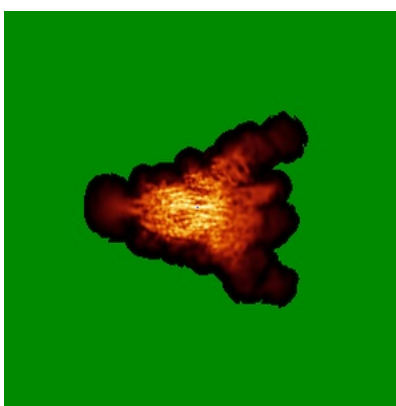
The images above show the largest variance slices of the map in three orthogonal directions.

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

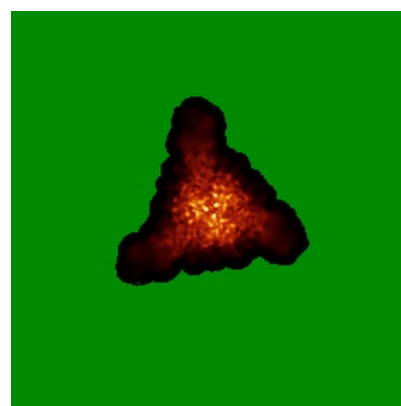
### 6.4.1 Primary map



X



Y

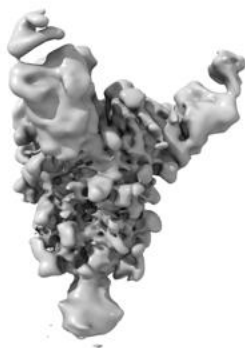


Z

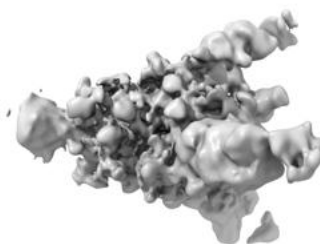
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

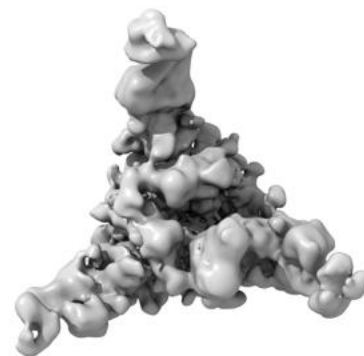
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

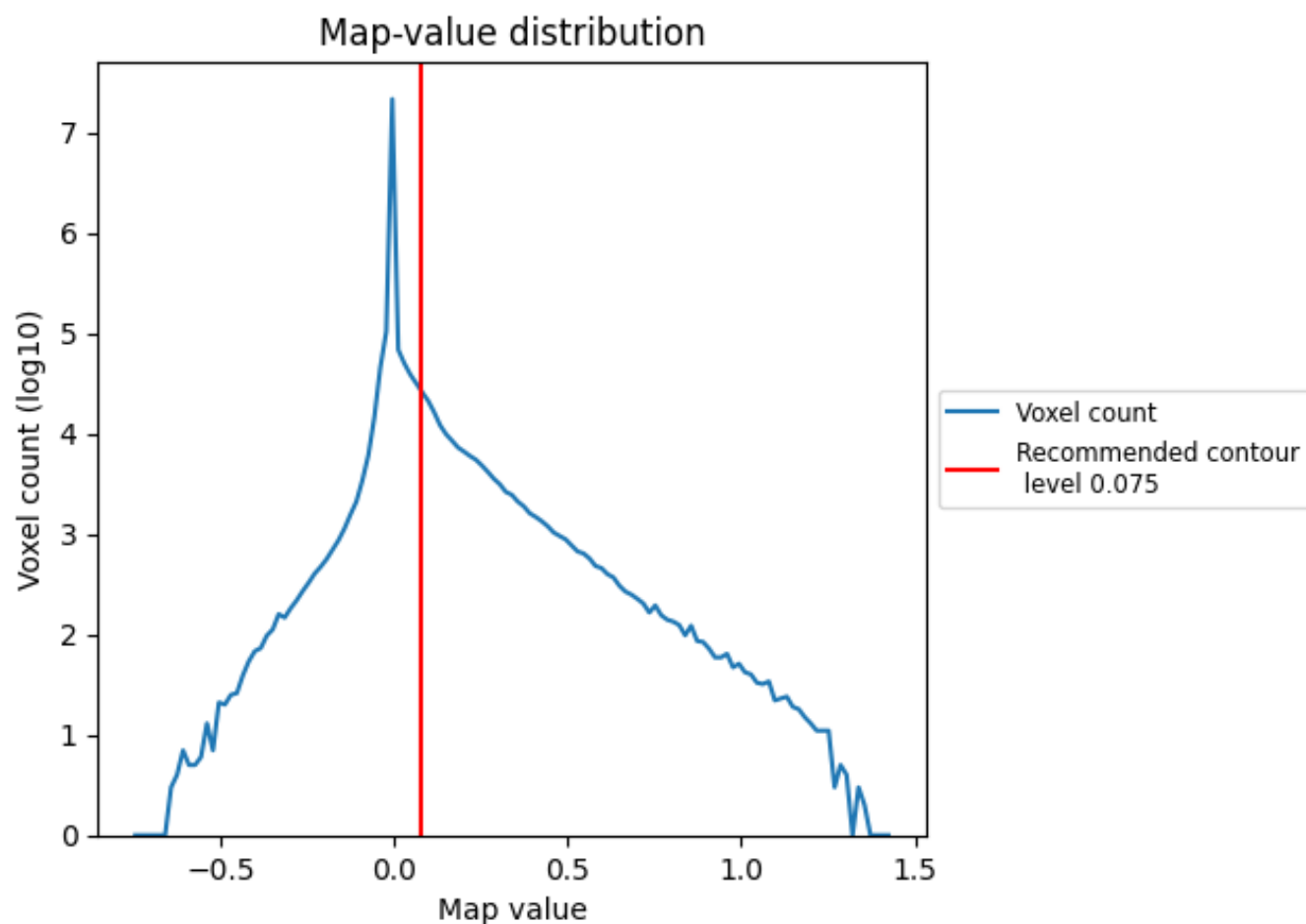
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

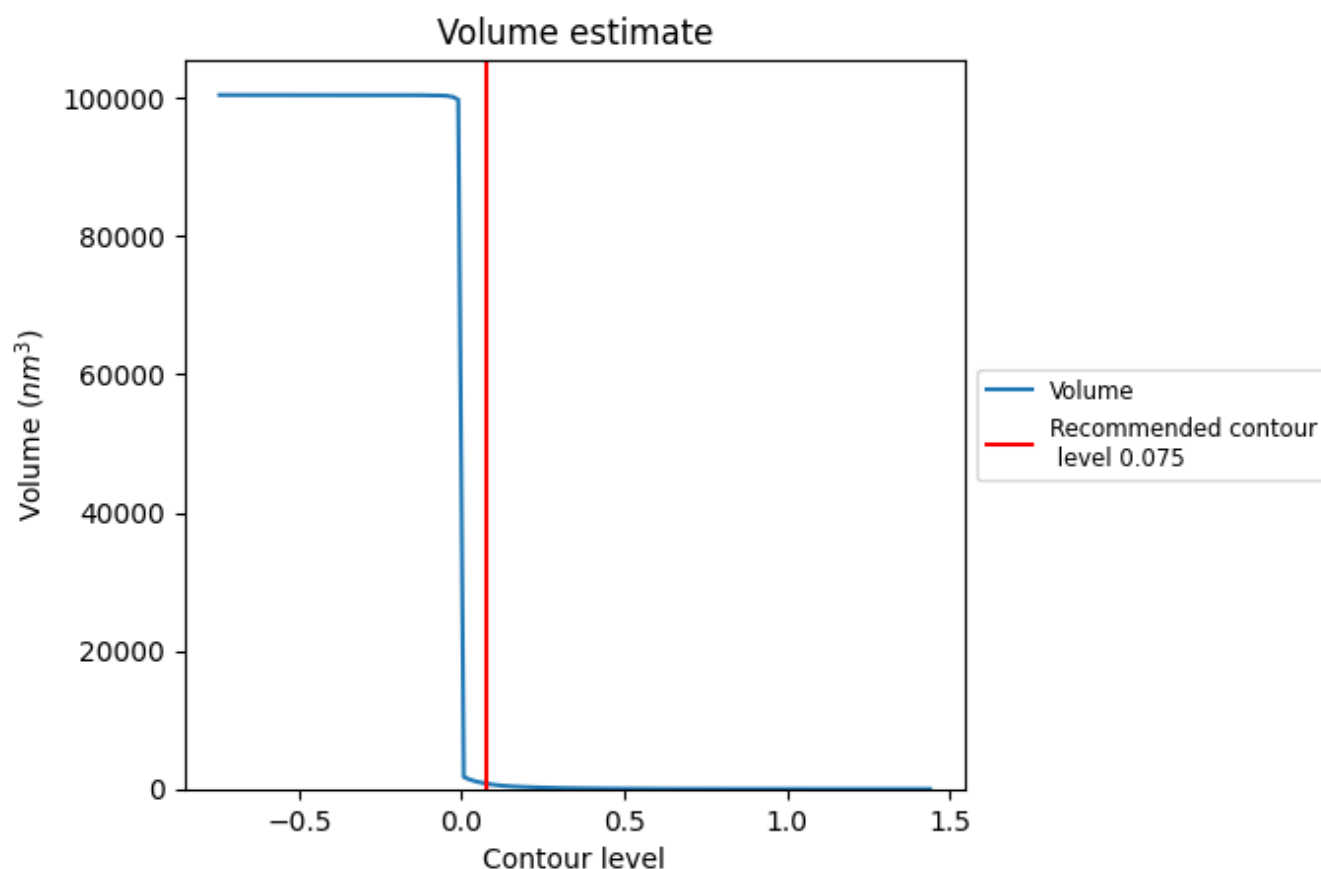
This section contains the results of statistical analysis of the map.

### 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](#)

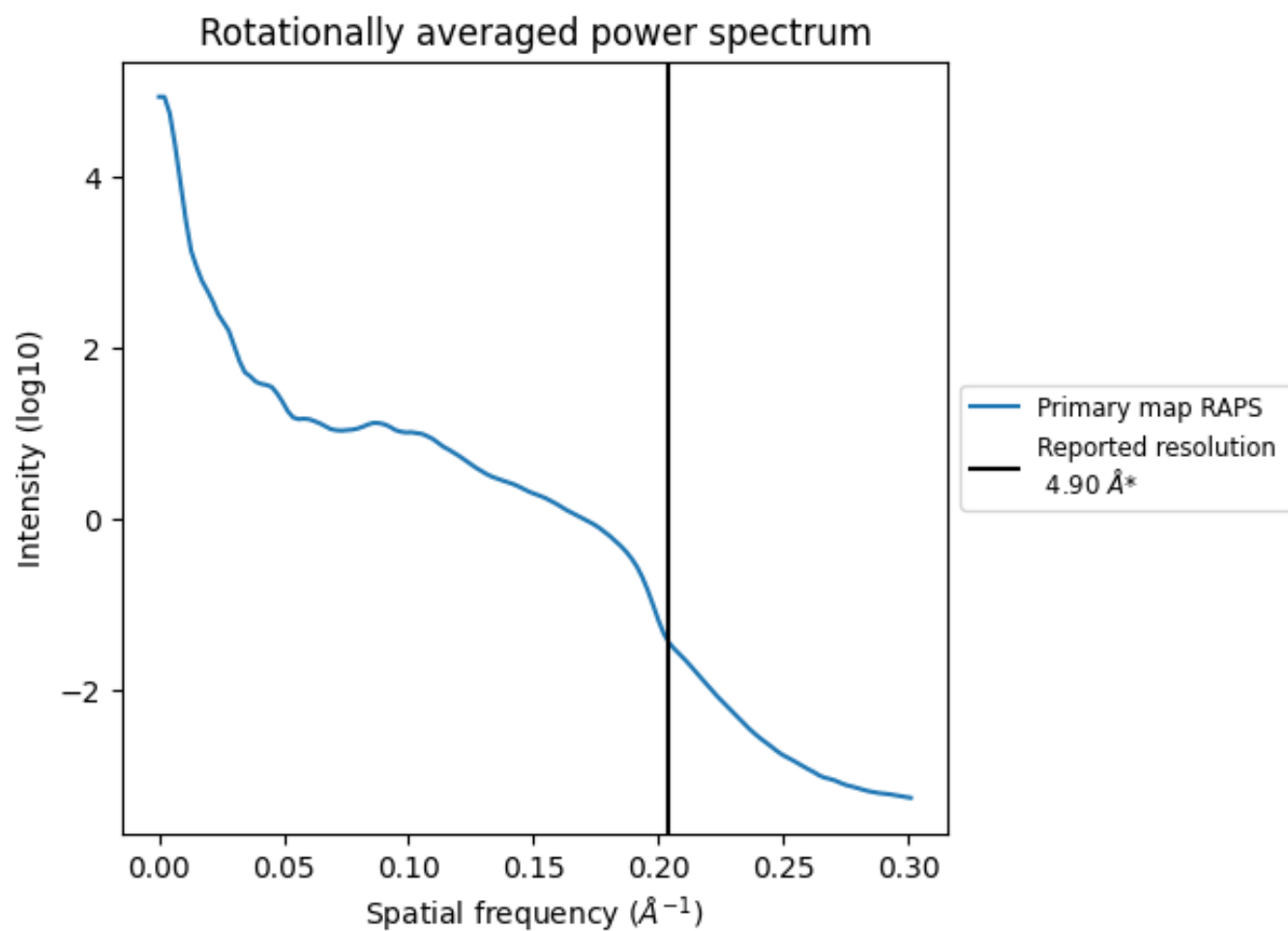


The volume at the recommended contour level is 782 nm<sup>3</sup>; this corresponds to an approximate mass of 707 kDa.

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 0.204 Å<sup>-1</sup>

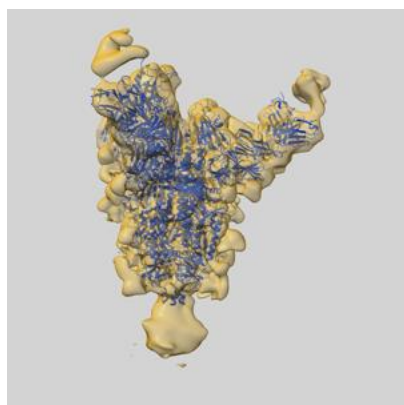
## 8 Fourier-Shell correlation

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

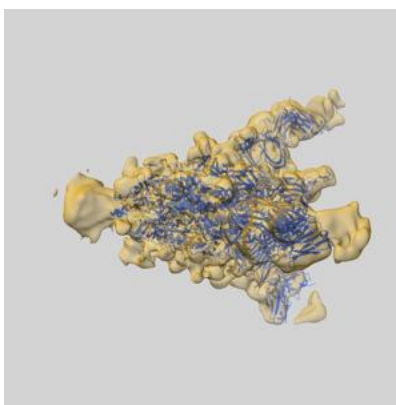
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13870 and PDB model 7Q9I. Per-residue inclusion information can be found in section 3 on page 15.

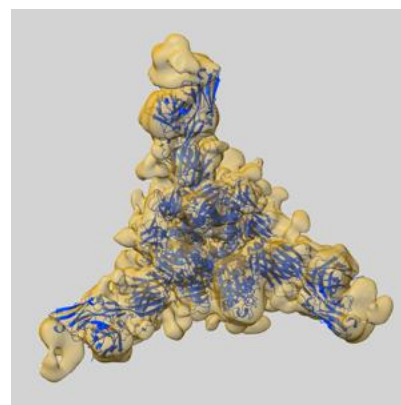
### 9.1 Map-model overlay [i](#)



X



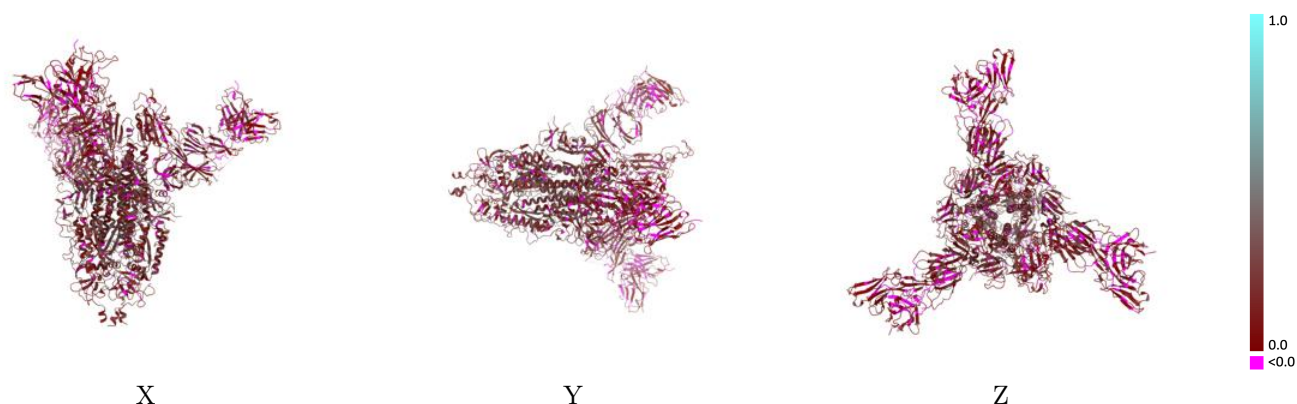
Y



Z

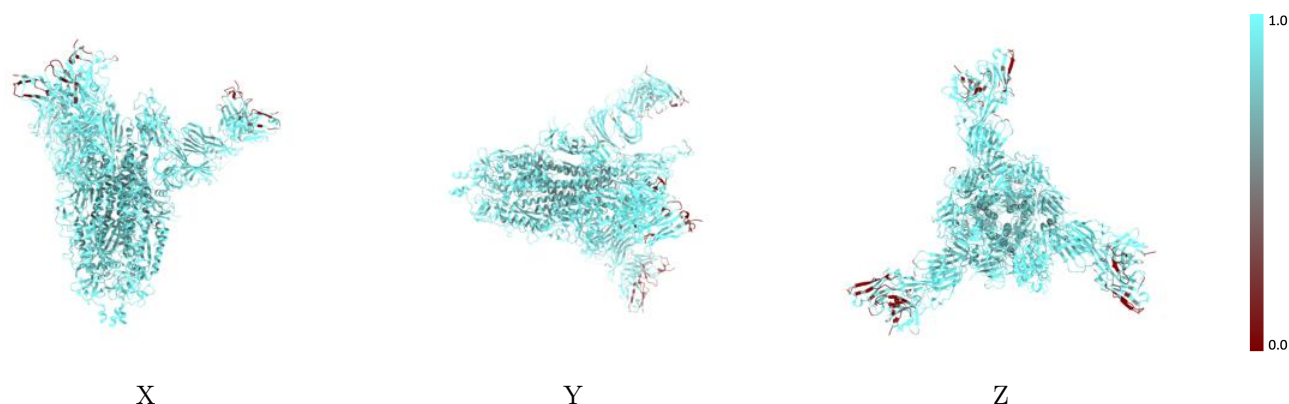
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



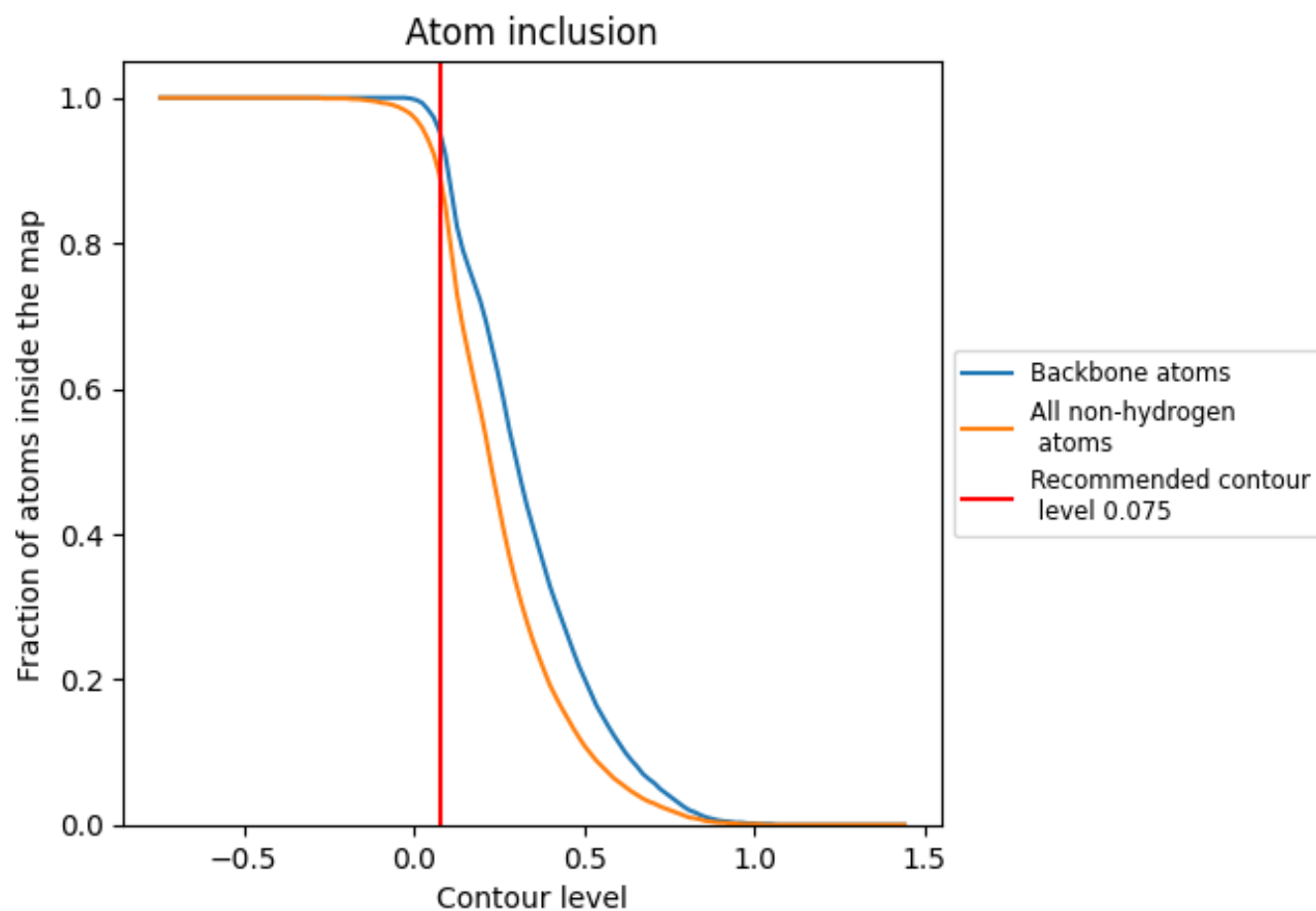
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 89% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8940	 0.1610
A	 0.9220	 0.1780
B	 0.9220	 0.1750
C	 0.9160	 0.1820
D	 0.9290	 0.3570
E	 0.7100	 0.0600
F	 0.7030	 0.0810
G	 1.0000	 0.2970
H	 0.8180	 0.0560
I	 1.0000	 0.2600
J	 0.7570	 0.0640
K	 0.7690	 0.0960
L	 0.8380	 0.0750
M	 1.0000	 0.3050
N	 1.0000	 0.3870
O	 0.9640	 0.2730
P	 1.0000	 0.2460
Q	 1.0000	 0.3130
R	 0.9640	 0.3370
S	 1.0000	 0.2830
T	 1.0000	 0.2640
U	 1.0000	 0.2980

