



## Full wwPDB EM Validation Report ⓘ

Jan 26, 2025 – 05:00 PM JST

PDB ID : 8Z7L  
EMDB ID : EMD-39819  
Title : Cryo-EM structure of SARS-CoV-2 S trimer in the early fusion intermediate conformation (E-FIC) (focused refinement of S-bottom)  
Authors : Liu, Z.; Xing, L.  
Deposited on : 2024-04-20  
Resolution : 3.42 Å(reported)

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 : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

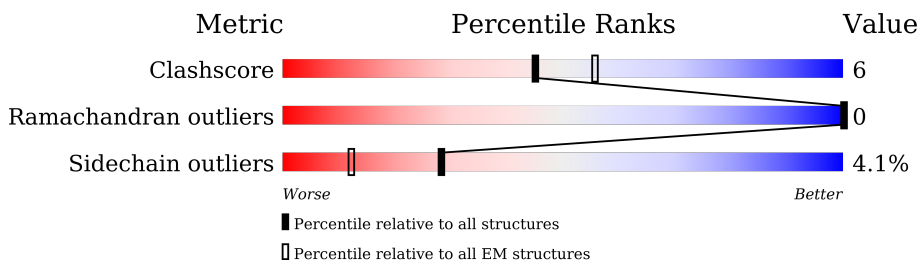
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.42 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	1288	
1	B	1288	
1	C	1288	
2	D	2	
2	E	2	
2	F	2	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6774 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	281	Total	C	N	O	S	0	0
			2202	1408	362	423	9		
1	B	281	Total	C	N	O	S	0	0
			2202	1408	362	423	9		
1	C	281	Total	C	N	O	S	0	0
			2202	1408	362	423	9		

There are 243 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	614	GLY	ASP	variant	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1232	PHE	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	GLY	-	expression tag	UNP P0DTC2
A	1240	LEU	-	expression tag	UNP P0DTC2
A	1241	GLU	-	expression tag	UNP P0DTC2
A	1242	VAL	-	expression tag	UNP P0DTC2
A	1243	LEU	-	expression tag	UNP P0DTC2
A	1244	PHE	-	expression tag	UNP P0DTC2
A	1245	GLN	-	expression tag	UNP P0DTC2
A	1246	GLY	-	expression tag	UNP P0DTC2
A	1247	PRO	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	TRP	-	expression tag	UNP P0DTC2
A	1251	SER	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	PRO	-	expression tag	UNP P0DTC2
A	1254	GLN	-	expression tag	UNP P0DTC2
A	1255	PHE	-	expression tag	UNP P0DTC2
A	1256	GLU	-	expression tag	UNP P0DTC2
A	1257	LYS	-	expression tag	UNP P0DTC2
A	1258	GLY	-	expression tag	UNP P0DTC2
A	1259	GLY	-	expression tag	UNP P0DTC2
A	1260	GLY	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	GLY	-	expression tag	UNP P0DTC2
A	1263	GLY	-	expression tag	UNP P0DTC2
A	1264	GLY	-	expression tag	UNP P0DTC2
A	1265	SER	-	expression tag	UNP P0DTC2
A	1266	GLY	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	ALA	-	expression tag	UNP P0DTC2
A	1270	TRP	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1274	GLN	-	expression tag	UNP P0DTC2
A	1275	PHE	-	expression tag	UNP P0DTC2
A	1276	GLU	-	expression tag	UNP P0DTC2
A	1277	LYS	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	GLY	-	expression tag	UNP P0DTC2
A	1280	SER	-	expression tag	UNP P0DTC2
A	1281	HIS	-	expression tag	UNP P0DTC2
A	1282	HIS	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	HIS	-	expression tag	UNP P0DTC2
A	1285	HIS	-	expression tag	UNP P0DTC2
A	1286	HIS	-	expression tag	UNP P0DTC2
A	1287	HIS	-	expression tag	UNP P0DTC2
A	1288	HIS	-	expression tag	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2
B	1221	GLN	-	expression tag	UNP P0DTC2
B	1222	ALA	-	expression tag	UNP P0DTC2
B	1223	TYR	-	expression tag	UNP P0DTC2
B	1224	VAL	-	expression tag	UNP P0DTC2
B	1225	ARG	-	expression tag	UNP P0DTC2
B	1226	LYS	-	expression tag	UNP P0DTC2
B	1227	ASP	-	expression tag	UNP P0DTC2
B	1228	GLY	-	expression tag	UNP P0DTC2
B	1229	GLU	-	expression tag	UNP P0DTC2
B	1230	TRP	-	expression tag	UNP P0DTC2
B	1231	VAL	-	expression tag	UNP P0DTC2
B	1232	PHE	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	GLY	-	expression tag	UNP P0DTC2
B	1240	LEU	-	expression tag	UNP P0DTC2
B	1241	GLU	-	expression tag	UNP P0DTC2
B	1242	VAL	-	expression tag	UNP P0DTC2
B	1243	LEU	-	expression tag	UNP P0DTC2
B	1244	PHE	-	expression tag	UNP P0DTC2
B	1245	GLN	-	expression tag	UNP P0DTC2
B	1246	GLY	-	expression tag	UNP P0DTC2
B	1247	PRO	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2
B	1249	GLY	-	expression tag	UNP P0DTC2
B	1250	TRP	-	expression tag	UNP P0DTC2
B	1251	SER	-	expression tag	UNP P0DTC2
B	1252	HIS	-	expression tag	UNP P0DTC2
B	1253	PRO	-	expression tag	UNP P0DTC2
B	1254	GLN	-	expression tag	UNP P0DTC2
B	1255	PHE	-	expression tag	UNP P0DTC2
B	1256	GLU	-	expression tag	UNP P0DTC2
B	1257	LYS	-	expression tag	UNP P0DTC2
B	1258	GLY	-	expression tag	UNP P0DTC2
B	1259	GLY	-	expression tag	UNP P0DTC2
B	1260	GLY	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	GLY	-	expression tag	UNP P0DTC2
B	1263	GLY	-	expression tag	UNP P0DTC2
B	1264	GLY	-	expression tag	UNP P0DTC2
B	1265	SER	-	expression tag	UNP P0DTC2
B	1266	GLY	-	expression tag	UNP P0DTC2
B	1267	GLY	-	expression tag	UNP P0DTC2
B	1268	SER	-	expression tag	UNP P0DTC2
B	1269	ALA	-	expression tag	UNP P0DTC2
B	1270	TRP	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	HIS	-	expression tag	UNP P0DTC2
B	1273	PRO	-	expression tag	UNP P0DTC2
B	1274	GLN	-	expression tag	UNP P0DTC2
B	1275	PHE	-	expression tag	UNP P0DTC2
B	1276	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1277	LYS	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	GLY	-	expression tag	UNP P0DTC2
B	1280	SER	-	expression tag	UNP P0DTC2
B	1281	HIS	-	expression tag	UNP P0DTC2
B	1282	HIS	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	HIS	-	expression tag	UNP P0DTC2
B	1285	HIS	-	expression tag	UNP P0DTC2
B	1286	HIS	-	expression tag	UNP P0DTC2
B	1287	HIS	-	expression tag	UNP P0DTC2
B	1288	HIS	-	expression tag	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	TYR	-	expression tag	UNP P0DTC2
C	1213	ILE	-	expression tag	UNP P0DTC2
C	1214	PRO	-	expression tag	UNP P0DTC2
C	1215	GLU	-	expression tag	UNP P0DTC2
C	1216	ALA	-	expression tag	UNP P0DTC2
C	1217	PRO	-	expression tag	UNP P0DTC2
C	1218	ARG	-	expression tag	UNP P0DTC2
C	1219	ASP	-	expression tag	UNP P0DTC2
C	1220	GLY	-	expression tag	UNP P0DTC2
C	1221	GLN	-	expression tag	UNP P0DTC2
C	1222	ALA	-	expression tag	UNP P0DTC2
C	1223	TYR	-	expression tag	UNP P0DTC2
C	1224	VAL	-	expression tag	UNP P0DTC2
C	1225	ARG	-	expression tag	UNP P0DTC2
C	1226	LYS	-	expression tag	UNP P0DTC2
C	1227	ASP	-	expression tag	UNP P0DTC2
C	1228	GLY	-	expression tag	UNP P0DTC2
C	1229	GLU	-	expression tag	UNP P0DTC2
C	1230	TRP	-	expression tag	UNP P0DTC2
C	1231	VAL	-	expression tag	UNP P0DTC2
C	1232	PHE	-	expression tag	UNP P0DTC2
C	1233	LEU	-	expression tag	UNP P0DTC2
C	1234	SER	-	expression tag	UNP P0DTC2
C	1235	THR	-	expression tag	UNP P0DTC2
C	1236	PHE	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	GLY	-	expression tag	UNP P0DTC2
C	1240	LEU	-	expression tag	UNP P0DTC2
C	1241	GLU	-	expression tag	UNP P0DTC2
C	1242	VAL	-	expression tag	UNP P0DTC2
C	1243	LEU	-	expression tag	UNP P0DTC2
C	1244	PHE	-	expression tag	UNP P0DTC2
C	1245	GLN	-	expression tag	UNP P0DTC2
C	1246	GLY	-	expression tag	UNP P0DTC2
C	1247	PRO	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	GLY	-	expression tag	UNP P0DTC2
C	1250	TRP	-	expression tag	UNP P0DTC2
C	1251	SER	-	expression tag	UNP P0DTC2
C	1252	HIS	-	expression tag	UNP P0DTC2
C	1253	PRO	-	expression tag	UNP P0DTC2
C	1254	GLN	-	expression tag	UNP P0DTC2
C	1255	PHE	-	expression tag	UNP P0DTC2
C	1256	GLU	-	expression tag	UNP P0DTC2
C	1257	LYS	-	expression tag	UNP P0DTC2
C	1258	GLY	-	expression tag	UNP P0DTC2
C	1259	GLY	-	expression tag	UNP P0DTC2
C	1260	GLY	-	expression tag	UNP P0DTC2
C	1261	SER	-	expression tag	UNP P0DTC2
C	1262	GLY	-	expression tag	UNP P0DTC2
C	1263	GLY	-	expression tag	UNP P0DTC2
C	1264	GLY	-	expression tag	UNP P0DTC2
C	1265	SER	-	expression tag	UNP P0DTC2
C	1266	GLY	-	expression tag	UNP P0DTC2
C	1267	GLY	-	expression tag	UNP P0DTC2
C	1268	SER	-	expression tag	UNP P0DTC2
C	1269	ALA	-	expression tag	UNP P0DTC2
C	1270	TRP	-	expression tag	UNP P0DTC2
C	1271	SER	-	expression tag	UNP P0DTC2
C	1272	HIS	-	expression tag	UNP P0DTC2
C	1273	PRO	-	expression tag	UNP P0DTC2
C	1274	GLN	-	expression tag	UNP P0DTC2
C	1275	PHE	-	expression tag	UNP P0DTC2
C	1276	GLU	-	expression tag	UNP P0DTC2
C	1277	LYS	-	expression tag	UNP P0DTC2
C	1278	GLY	-	expression tag	UNP P0DTC2
C	1279	GLY	-	expression tag	UNP P0DTC2

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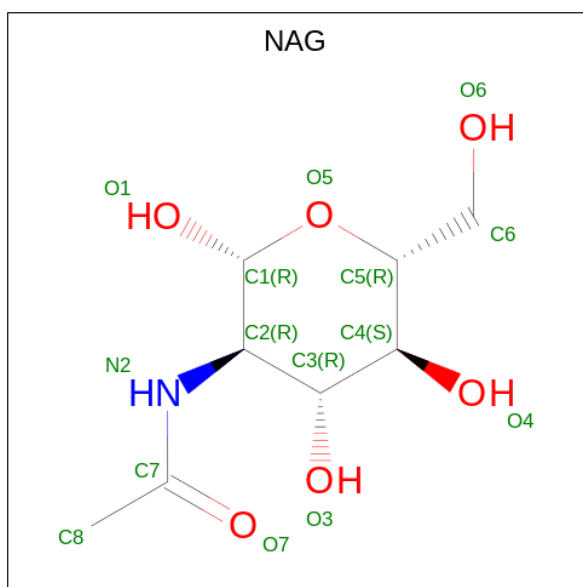
Chain	Residue	Modelled	Actual	Comment	Reference
C	1280	SER	-	expression tag	UNP P0DTC2
C	1281	HIS	-	expression tag	UNP P0DTC2
C	1282	HIS	-	expression tag	UNP P0DTC2
C	1283	HIS	-	expression tag	UNP P0DTC2
C	1284	HIS	-	expression tag	UNP P0DTC2
C	1285	HIS	-	expression tag	UNP P0DTC2
C	1286	HIS	-	expression tag	UNP P0DTC2
C	1287	HIS	-	expression tag	UNP P0DTC2
C	1288	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		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

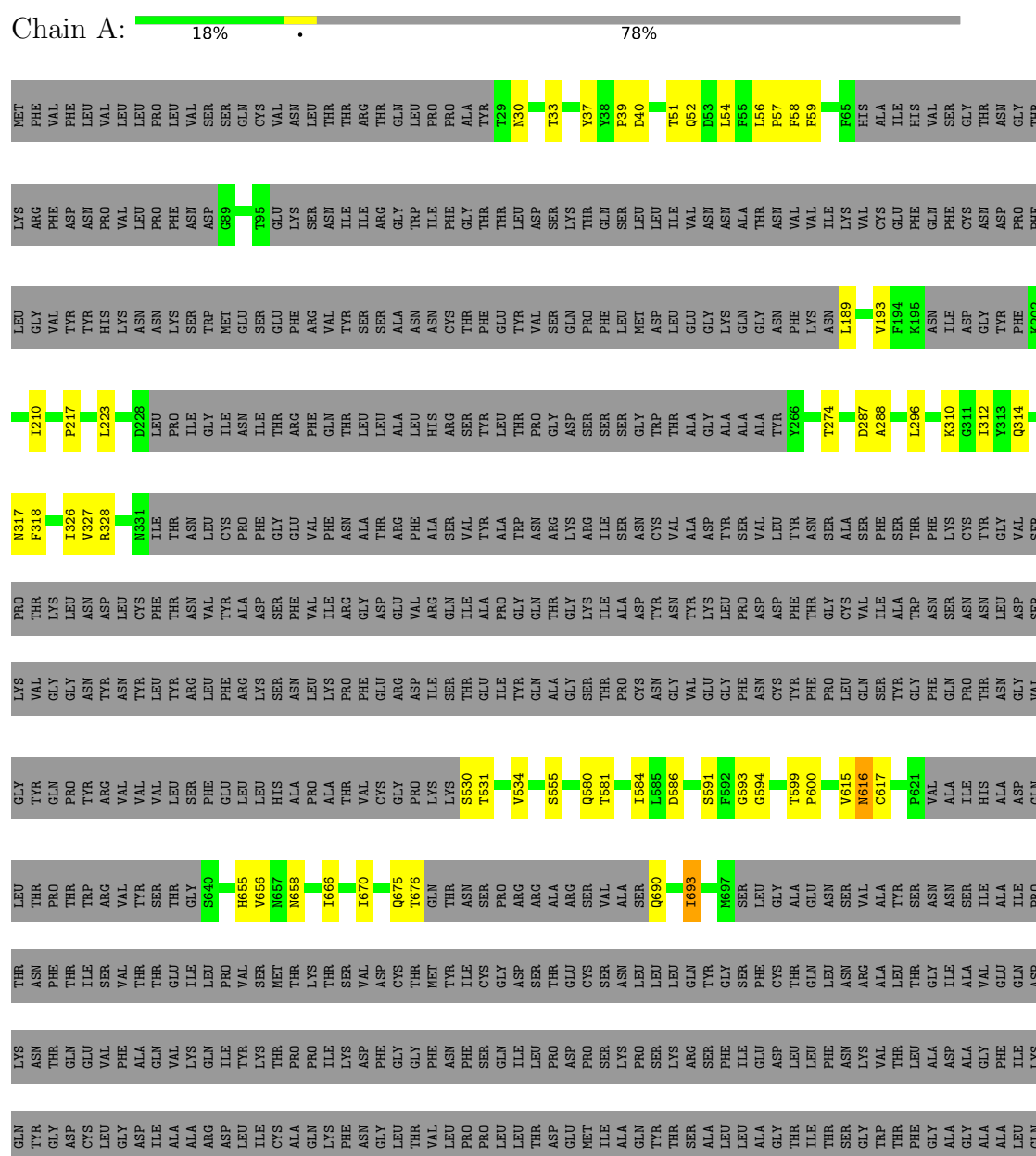


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

### 3 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.

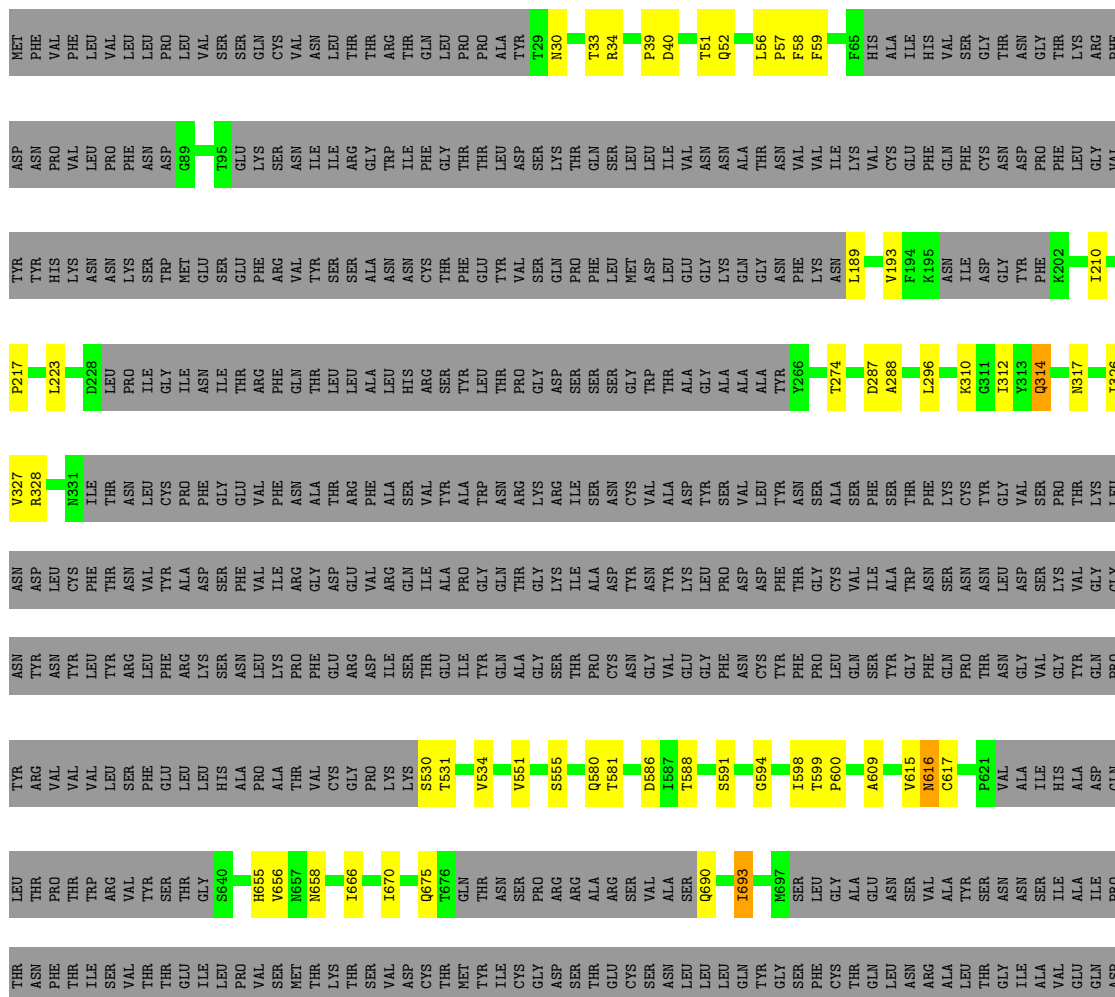
#### • Molecule 1: Spike glycoprotein



[illegible]

- Molecule 1: Spike glycoprotein

Chain B:  18% . 78%



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

- Molecule 1: Spike glycoprotein

Chain C:  18% 2% 80%

[illegible]



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	97415	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	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	16.465	Depositor
Minimum map value	-0.139	Depositor
Average map value	-0.048	Depositor
Map value standard deviation	0.260	Depositor
Recommended contour level	1	Depositor
Map size (Å)	372.8, 372.8, 372.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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	0.24	0/2247	0.43	0/3051
1	B	0.24	0/2247	0.43	0/3051
1	C	0.25	0/2247	0.43	0/3051
All	All	0.24	0/6741	0.43	0/9153

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	2202	0	2139	27	0
1	B	2202	0	2139	26	0
1	C	2202	0	2139	28	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
All	All	6774	0	6570	81	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 6.

All (81) 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:555:SER:HB2	1:B:586:ASP:HB2	1.76	0.68
1:C:317:ASN:HA	1:C:594:GLY:HA2	1.78	0.66
1:C:555:SER:HB2	1:C:586:ASP:HB2	1.77	0.66
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.78	0.65
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.78	0.65
1:B:317:ASN:HA	1:B:594:GLY:HA2	1.79	0.65
1:A:52:GLN:NE2	1:A:274:THR:OG1	2.35	0.60
1:B:52:GLN:NE2	1:B:274:THR:OG1	2.36	0.59
1:C:52:GLN:NE2	1:C:274:THR:OG1	2.36	0.58
1:C:328:ARG:NH2	1:C:531:THR:O	2.35	0.57
1:B:328:ARG:NH2	1:B:531:THR:O	2.37	0.56
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.87	0.56
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.87	0.56
1:C:56:LEU:HD12	1:C:57:PRO:HD2	1.87	0.55
1:A:328:ARG:NH2	1:A:531:THR:O	2.38	0.55
1:C:326:ILE:HD13	1:C:534:VAL:HG12	1.91	0.53
1:B:189:LEU:HD22	1:B:217:PRO:HG2	1.91	0.53
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.90	0.53
1:C:656:VAL:HG12	1:C:658:ASN:H	1.73	0.53
1:C:591:SER:HB3	1:C:615:VAL:HG12	1.90	0.53
1:B:656:VAL:HG12	1:B:658:ASN:H	1.74	0.52
1:A:189:LEU:HD22	1:A:217:PRO:HG2	1.91	0.52
1:B:326:ILE:HD13	1:B:534:VAL:HG12	1.90	0.52
1:C:327:VAL:O	1:C:530:SER:N	2.42	0.52
1:A:326:ILE:HD13	1:A:534:VAL:HG12	1.91	0.52
1:B:328:ARG:NH1	1:B:580:GLN:OE1	2.43	0.52
1:A:656:VAL:HG12	1:A:658:ASN:H	1.74	0.52
1:A:327:VAL:O	1:A:530:SER:N	2.44	0.51
1:B:327:VAL:O	1:B:530:SER:N	2.43	0.51
1:C:193:VAL:HG23	1:C:223:LEU:HD22	1.92	0.51
1:A:328:ARG:NH1	1:A:580:GLN:OE1	2.44	0.51
1:B:591:SER:HB3	1:B:615:VAL:HG12	1.93	0.51
1:B:675:GLN:O	1:B:690:GLN:N	2.44	0.51
1:C:328:ARG:NH1	1:C:580:GLN:OE1	2.45	0.50
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.93	0.50
1:C:189:LEU:HD22	1:C:217:PRO:HG2	1.93	0.50
1:B:193:VAL:HG23	1:B:223:LEU:HD22	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ASN:HD21	1:C:59:PHE:HD1	1.59	0.50
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.93	0.50
1:A:193:VAL:HG23	1:A:223:LEU:HD22	1.93	0.49
1:A:591:SER:HB3	1:A:615:VAL:HG12	1.92	0.49
1:A:30:ASN:HD21	1:A:59:PHE:HD1	1.60	0.48
1:C:675:GLN:O	1:C:690:GLN:N	2.47	0.47
1:C:675:GLN:HB2	1:C:693:ILE:HD12	1.97	0.47
1:A:675:GLN:O	1:A:690:GLN:N	2.49	0.46
1:B:616:ASN:N	1:B:616:ASN:OD1	2.48	0.46
1:C:328:ARG:HH11	1:C:580:GLN:HB3	1.81	0.46
1:B:30:ASN:HD21	1:B:59:PHE:HD1	1.62	0.46
1:B:287:ASP:OD1	1:B:288:ALA:N	2.48	0.46
1:C:616:ASN:N	1:C:616:ASN:OD1	2.50	0.46
1:C:34:ARG:HH11	1:C:217:PRO:HB2	1.82	0.45
1:A:287:ASP:OD1	1:A:288:ALA:N	2.49	0.45
1:A:616:ASN:N	1:A:616:ASN:OD1	2.49	0.45
1:C:287:ASP:OD1	1:C:288:ALA:N	2.49	0.45
1:A:555:SER:HB3	1:A:584:ILE:HG13	1.99	0.45
1:A:189:LEU:HB2	1:A:210:ILE:HG12	1.99	0.44
1:B:314:GLN:HE21	1:B:314:GLN:HB3	1.63	0.44
1:B:598:ILE:HB	1:B:609:ALA:HB3	2.00	0.44
1:C:39:PRO:HG3	1:C:51:THR:HG21	2.00	0.43
1:A:675:GLN:HB2	1:A:693:ILE:HD12	2.01	0.43
1:A:328:ARG:HH11	1:A:580:GLN:HB3	1.84	0.43
1:B:328:ARG:HH11	1:B:580:GLN:HB3	1.83	0.43
1:C:189:LEU:HB2	1:C:210:ILE:HG12	2.01	0.43
1:A:318:PHE:N	1:A:593:GLY:O	2.52	0.43
1:C:676:THR:HG23	1:C:690:GLN:HG3	2.01	0.42
1:B:189:LEU:HB2	1:B:210:ILE:HG12	2.01	0.42
1:B:551:VAL:HG13	1:B:588:THR:HB	2.02	0.42
1:A:37:TYR:OH	1:A:54:LEU:O	2.33	0.42
1:A:39:PRO:HG3	1:A:51:THR:HG21	2.02	0.42
1:A:33:THR:HG22	1:A:58:PHE:CG	2.55	0.42
1:B:39:PRO:HG3	1:B:51:THR:HG21	2.02	0.42
1:B:675:GLN:HB2	1:B:693:ILE:HD12	2.01	0.42
1:B:666:ILE:HG12	1:B:670:ILE:O	2.20	0.41
1:A:676:THR:HG23	1:A:690:GLN:HG3	2.03	0.41
1:C:666:ILE:HG12	1:C:670:ILE:O	2.20	0.41
1:B:33:THR:HG22	1:B:58:PHE:CG	2.55	0.41
1:C:611:LEU:HD22	1:C:666:ILE:HB	2.02	0.41
1:C:33:THR:HG22	1:C:58:PHE:CG	2.56	0.41

*Continued on next page...*

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HG12	1:A:670:ILE:O	2.21	0.41
1:C:551:VAL:HG13	1:C:588:THR:HB	2.03	0.41
1:C:555:SER:HB3	1:C:584:ILE:HG13	2.03	0.41

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	265/1288 (21%)	252 (95%)	13 (5%)	0	100	100
1	B	265/1288 (21%)	252 (95%)	13 (5%)	0	100	100
1	C	265/1288 (21%)	252 (95%)	13 (5%)	0	100	100
All	All	795/3864 (21%)	756 (95%)	39 (5%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	251/1112 (23%)	241 (96%)	10 (4%)	27	52
1	B	251/1112 (23%)	240 (96%)	11 (4%)	24	50
1	C	251/1112 (23%)	241 (96%)	10 (4%)	27	52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	753/3336 (23%)	722 (96%)	31 (4%)	28 51

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

Mol	Chain	Res	Type
1	A	40	ASP
1	A	296	LEU
1	A	312	ILE
1	A	314	GLN
1	A	581	THR
1	A	599	THR
1	A	616	ASN
1	A	617	CYS
1	A	655	HIS
1	A	693	ILE
1	B	34	ARG
1	B	40	ASP
1	B	296	LEU
1	B	312	ILE
1	B	314	GLN
1	B	581	THR
1	B	599	THR
1	B	616	ASN
1	B	617	CYS
1	B	655	HIS
1	B	693	ILE
1	C	40	ASP
1	C	296	LEU
1	C	312	ILE
1	C	314	GLN
1	C	581	THR
1	C	599	THR
1	C	616	ASN
1	C	617	CYS
1	C	655	HIS
1	C	693	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN

*Continued on next page...*

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Mol	Chain	Res	Type
1	A	314	GLN
1	A	321	GLN
1	B	52	GLN
1	B	314	GLN
1	B	321	GLN
1	C	52	GLN
1	C	314	GLN
1	C	321	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

6 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	0.23	0	17,19,21	0.45	0
2	NAG	D	2	2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	E	1	1,2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	E	2	2	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	F	1	1,2	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	F	2	2	14,14,15	0.23	0	17,19,21	0.41	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	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

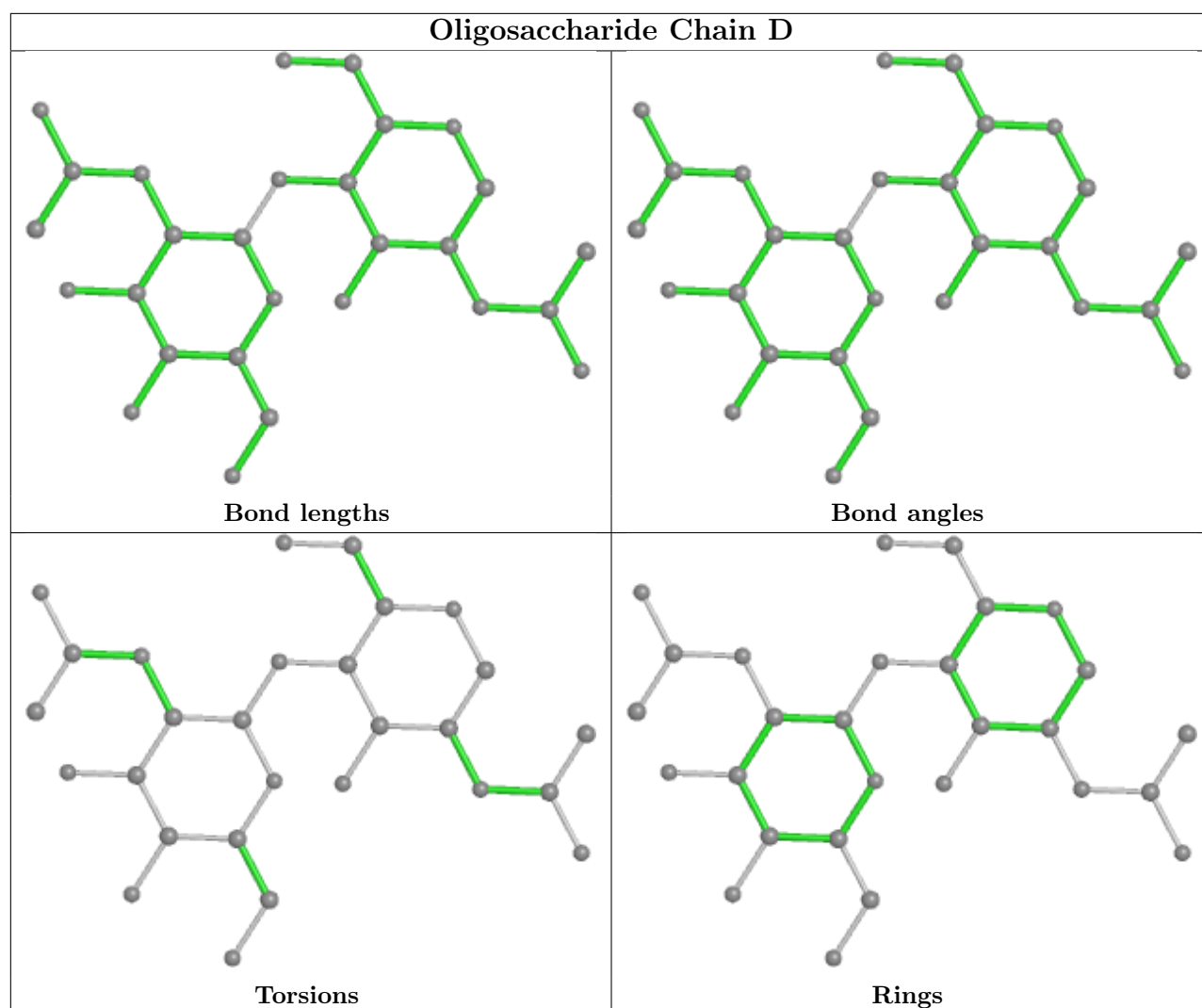
There are no torsion outliers.

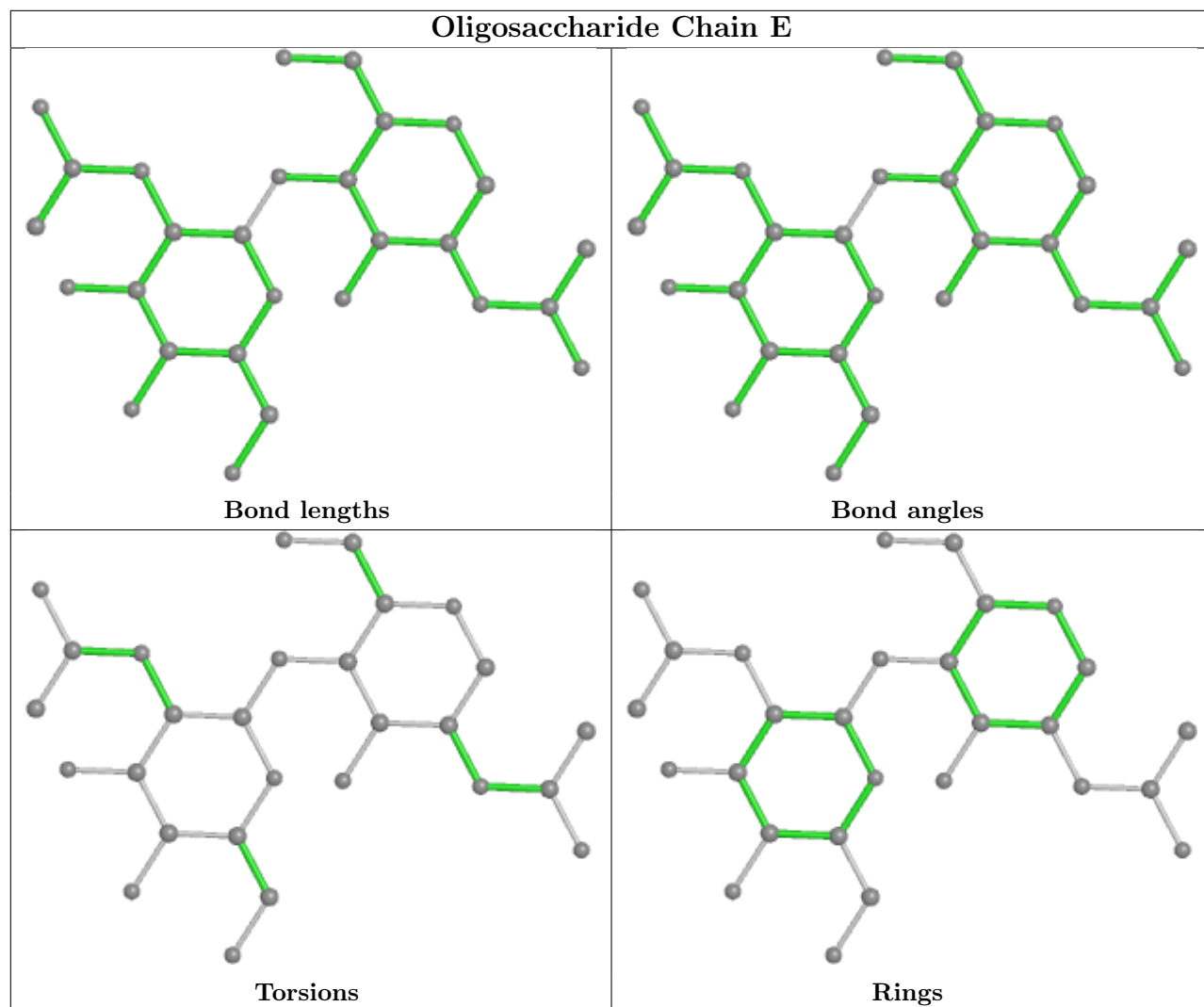
There are no ring outliers.

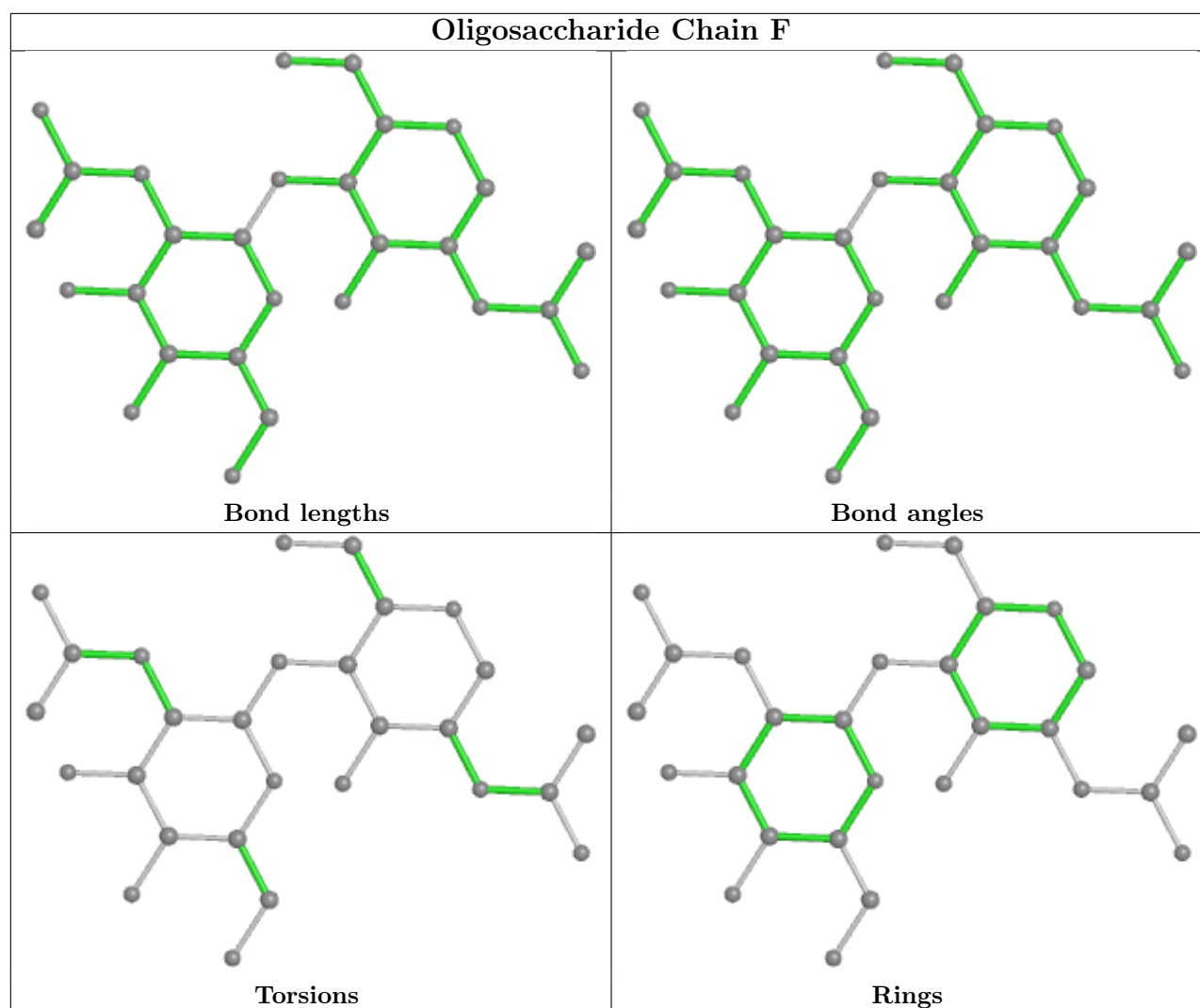
No monomer is involved in short contacts.

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](#)

6 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	1302	1	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	B	1301	1	14,14,15	0.20	0	17,19,21	0.44	0
3	NAG	A	1301	1	14,14,15	0.20	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.42	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
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	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 (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	B	1302	NAG	C4-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

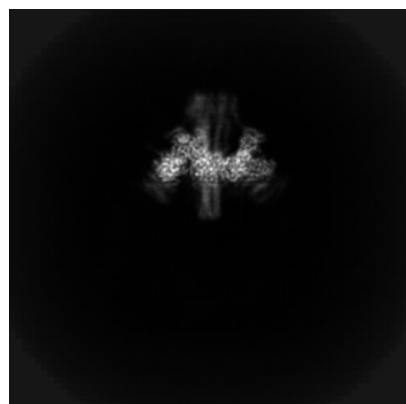
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39819. These allow visual inspection of the internal detail of the map and identification of artifacts.

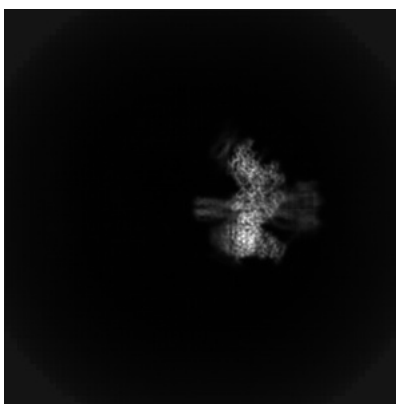
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

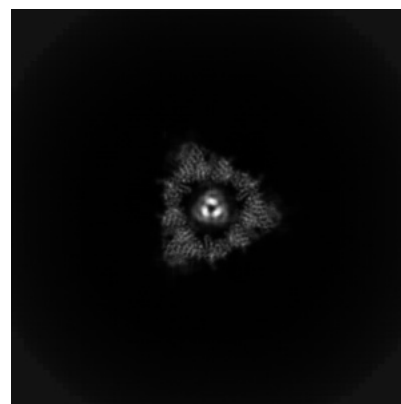
#### 6.1.1 Primary map



X

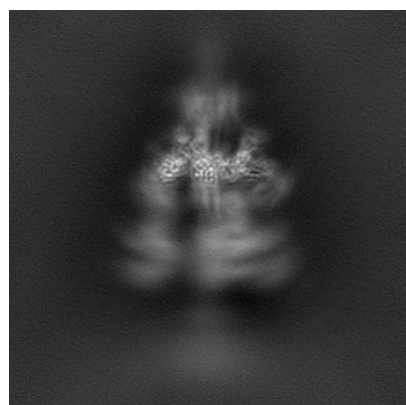


Y

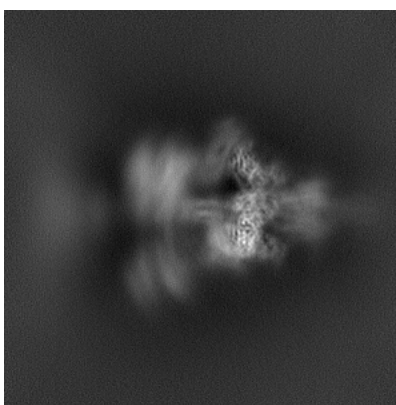


Z

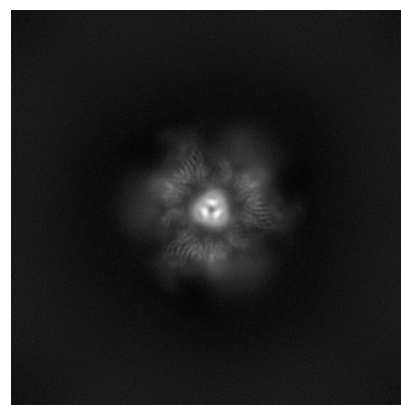
#### 6.1.2 Raw map



X



Y

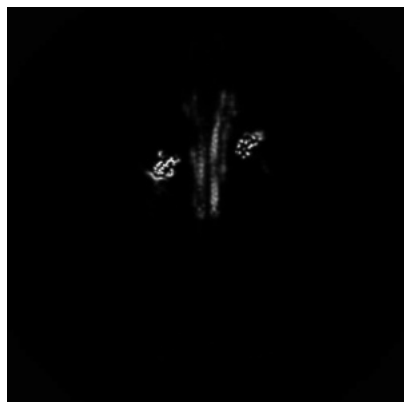


Z

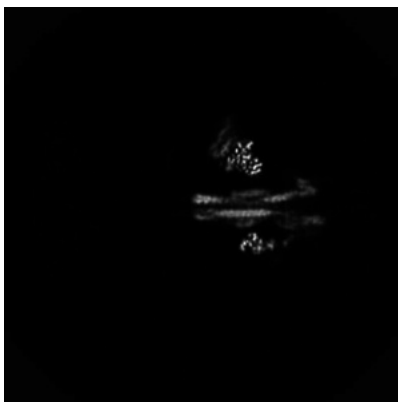
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

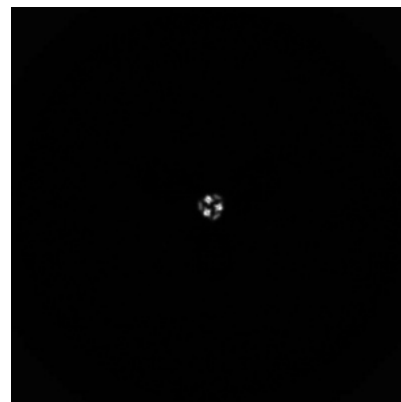
### 6.2.1 Primary map



X Index: 200



Y Index: 200

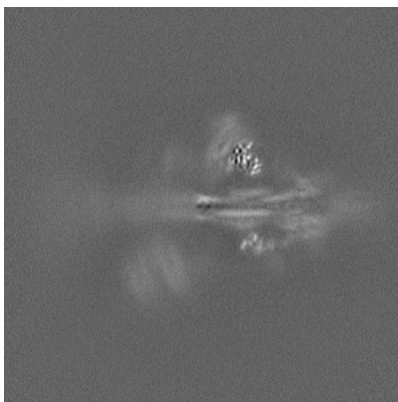


Z Index: 200

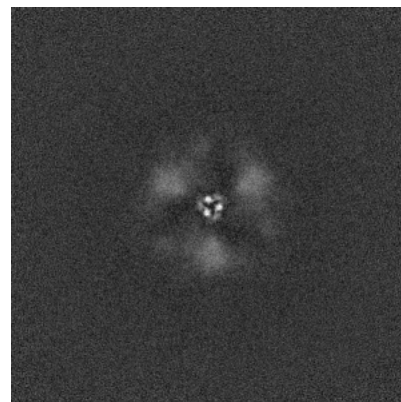
### 6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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

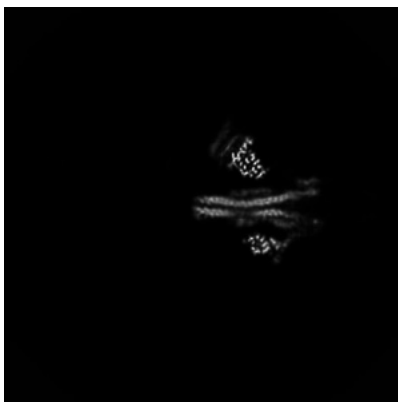


## 6.3 Largest variance slices [i](#)

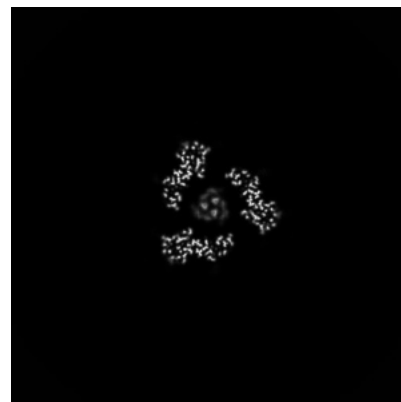
### 6.3.1 Primary map



X Index: 169

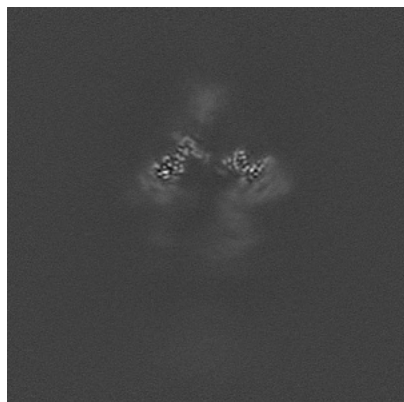


Y Index: 196

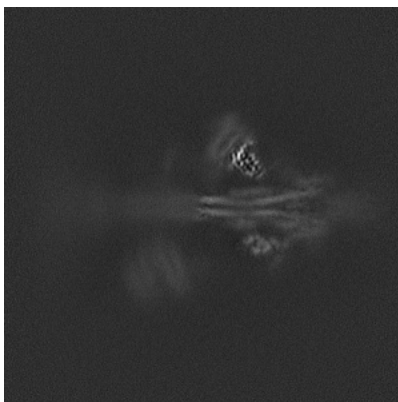


Z Index: 239

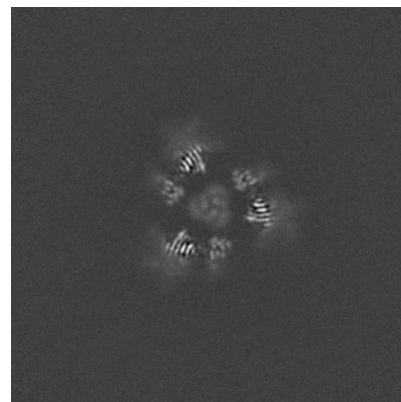
### 6.3.2 Raw map



X Index: 172



Y Index: 197



Z Index: 235

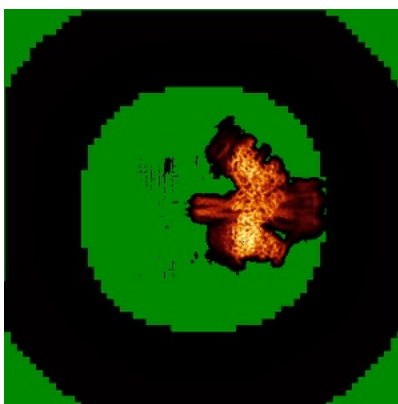
The images above show the largest variance slices of the map in three orthogonal directions.

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

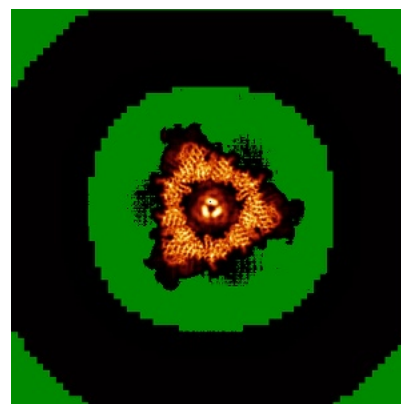
### 6.4.1 Primary map



X

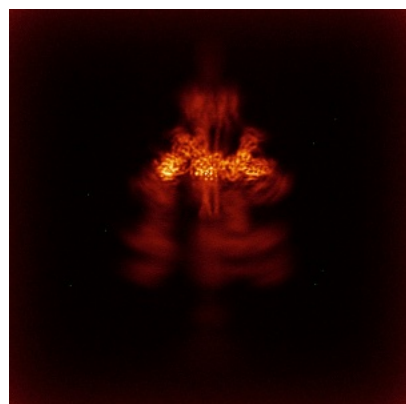


Y

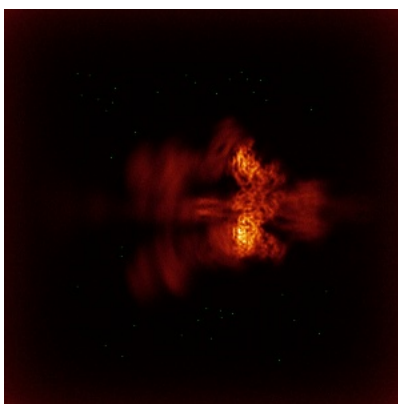


Z

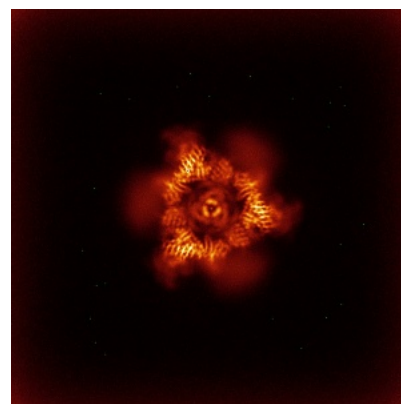
### 6.4.2 Raw map



X



Y

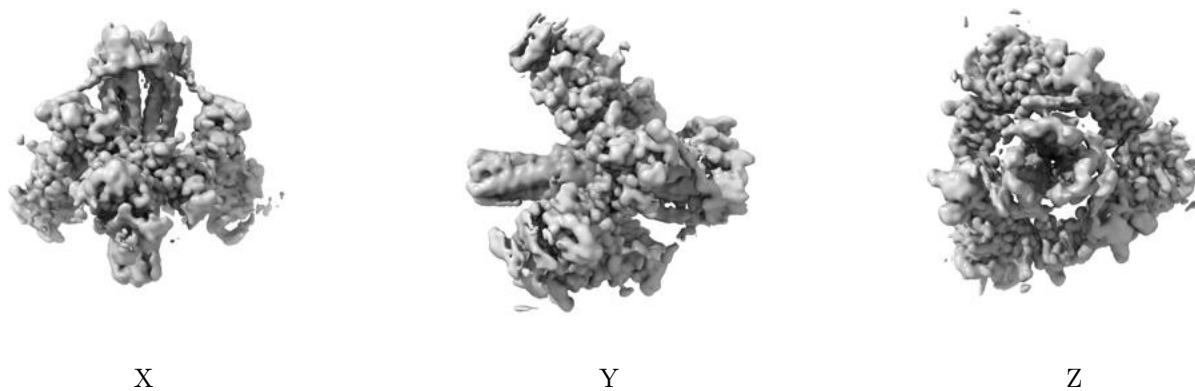


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

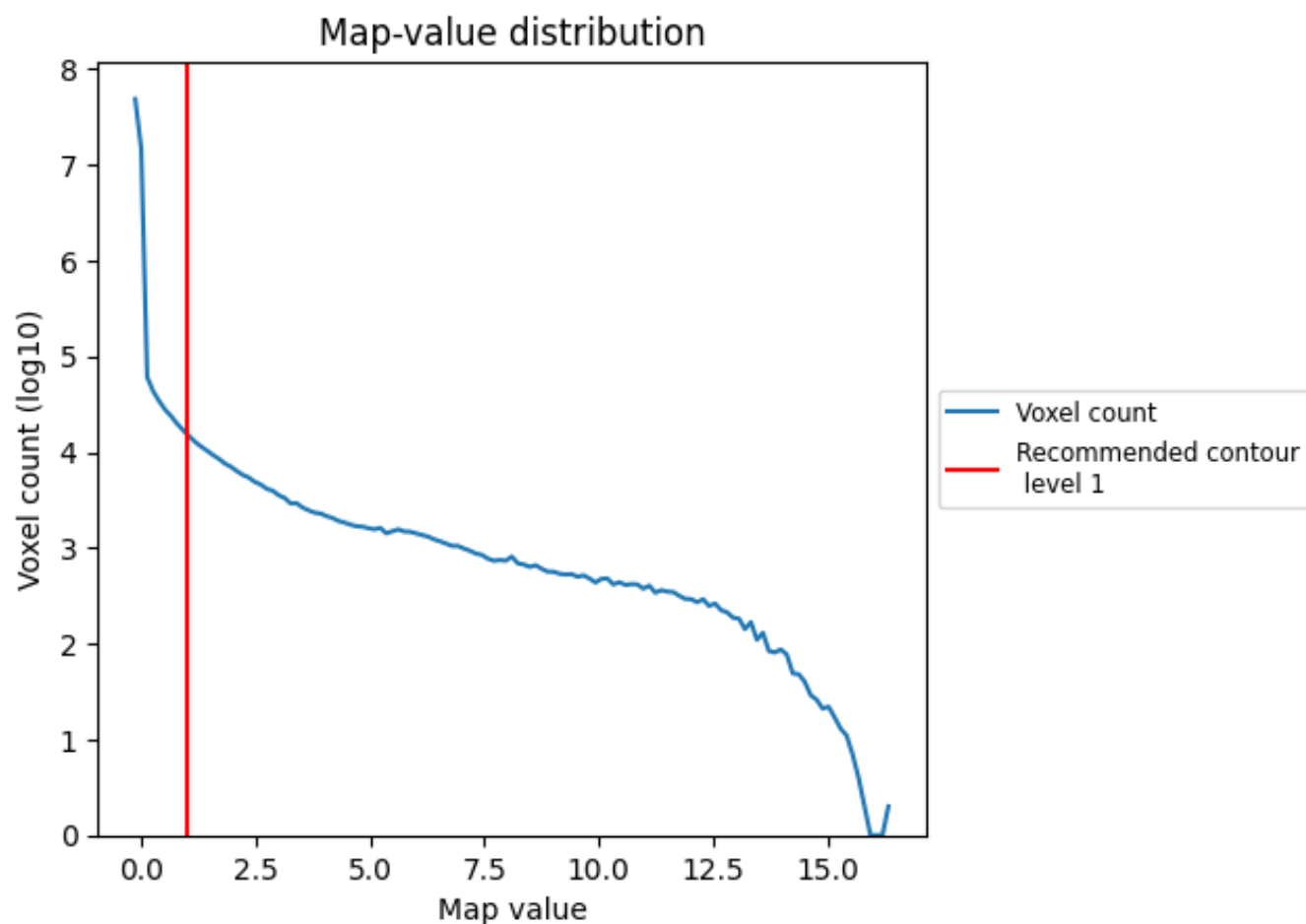
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

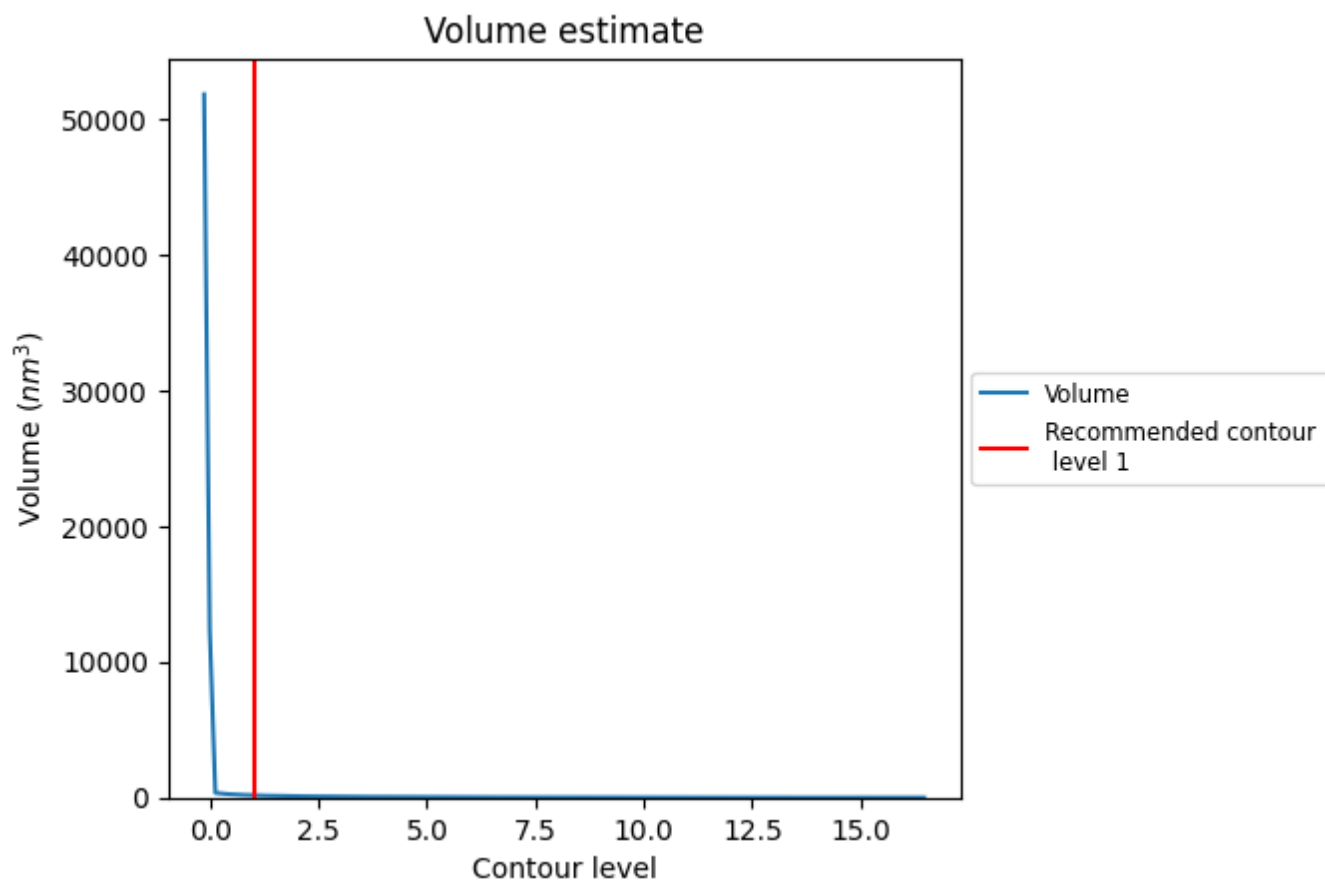
This section contains the results of statistical analysis of the map.

### 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.

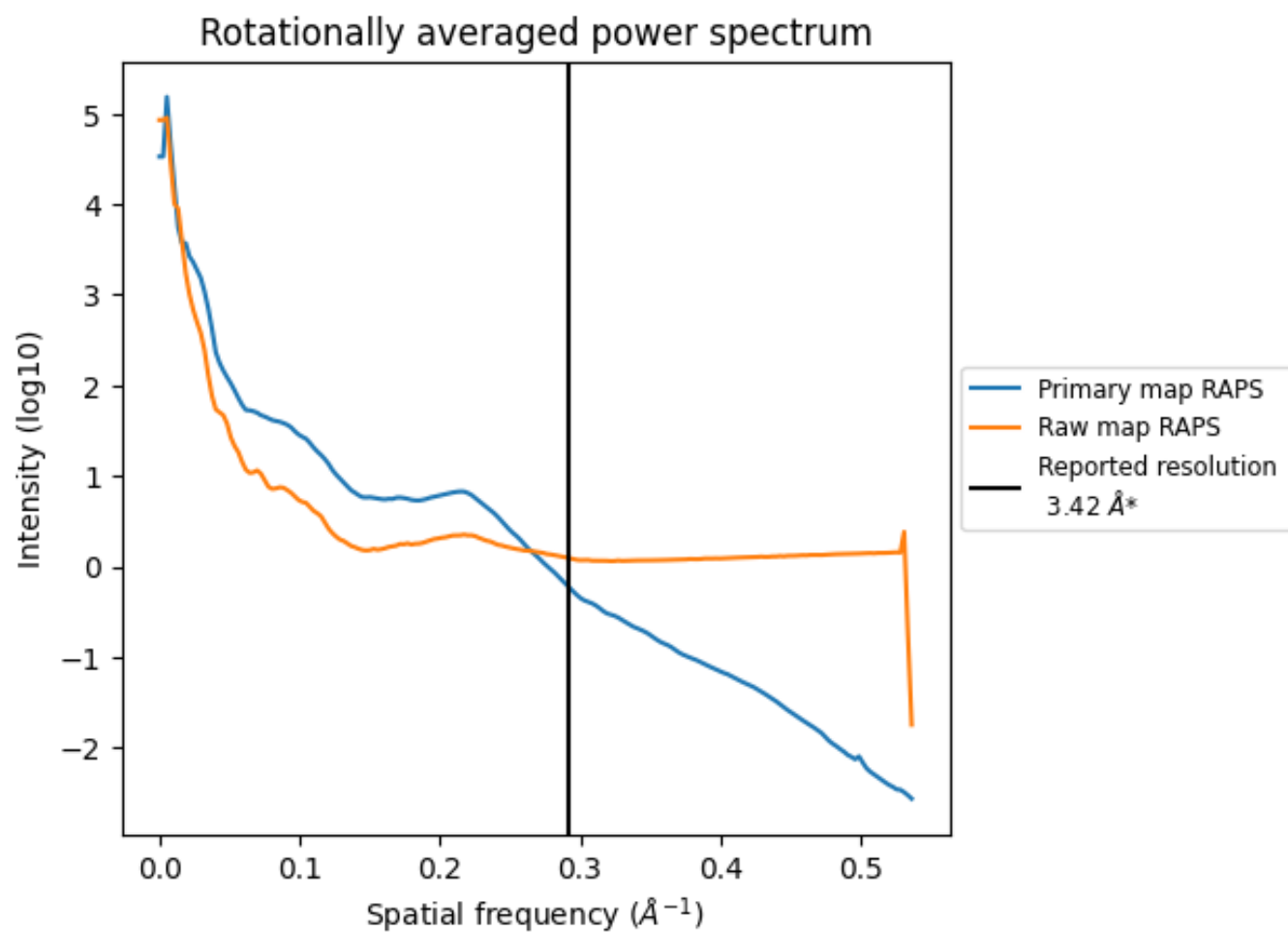
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165 nm<sup>3</sup>; this corresponds to an approximate mass of 149 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

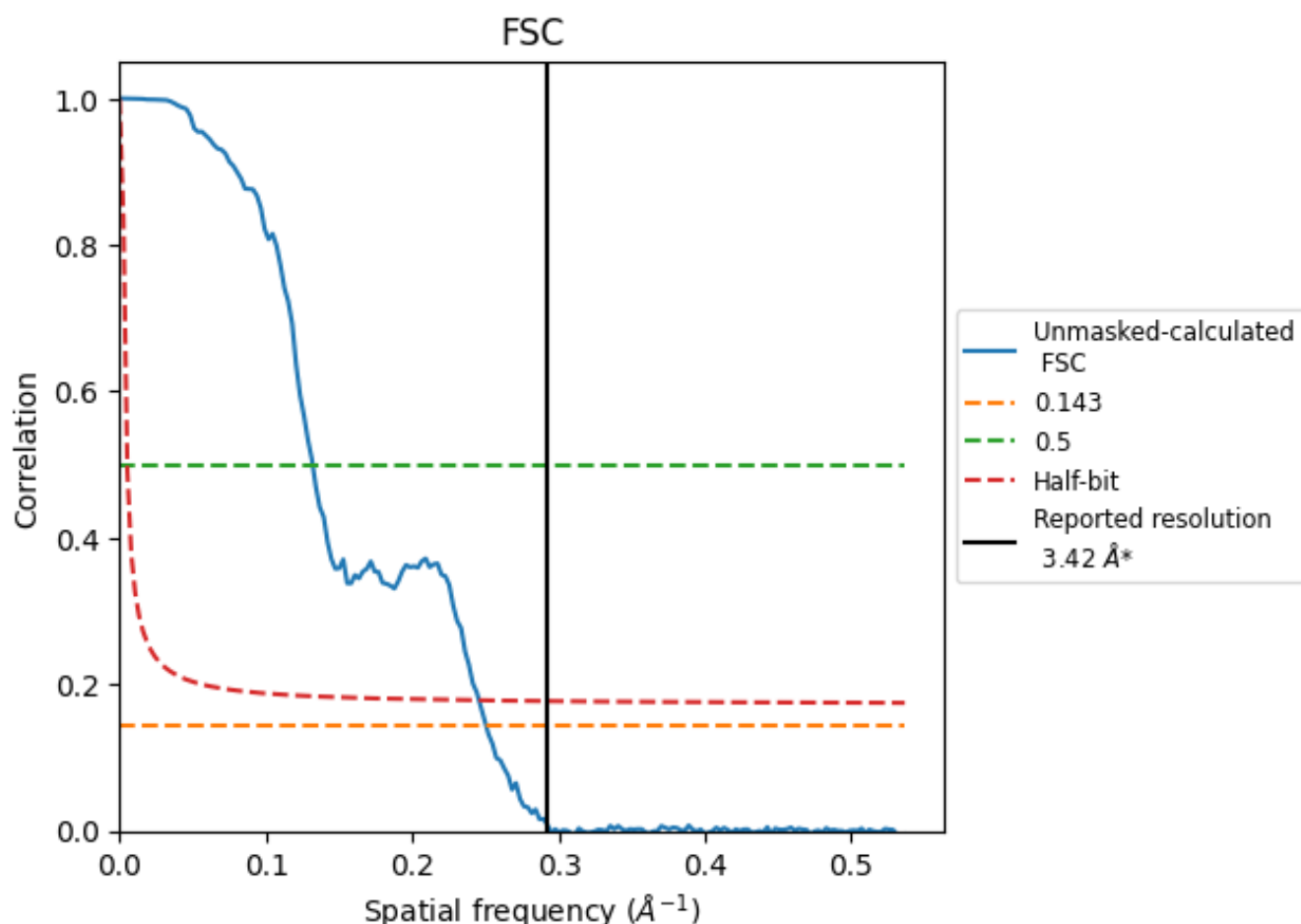


\*Reported resolution corresponds to spatial frequency of  $0.292 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.292  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

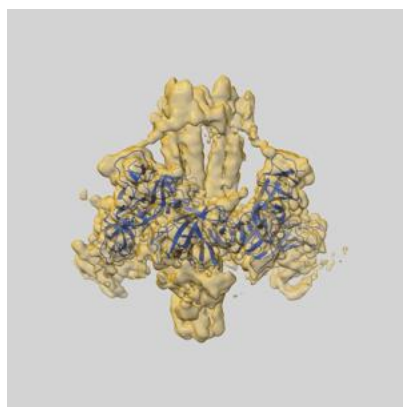
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.42	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	7.58	4.07

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.42 by more than 10 %

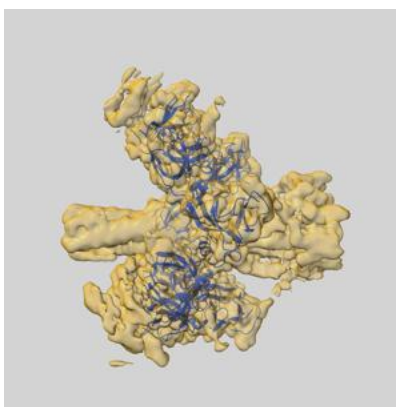
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39819 and PDB model 8Z7L. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

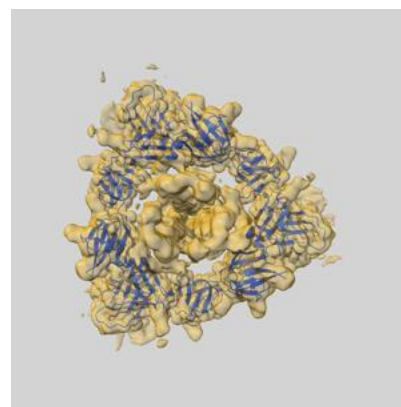
### 9.1 Map-model overlay [i](#)



X



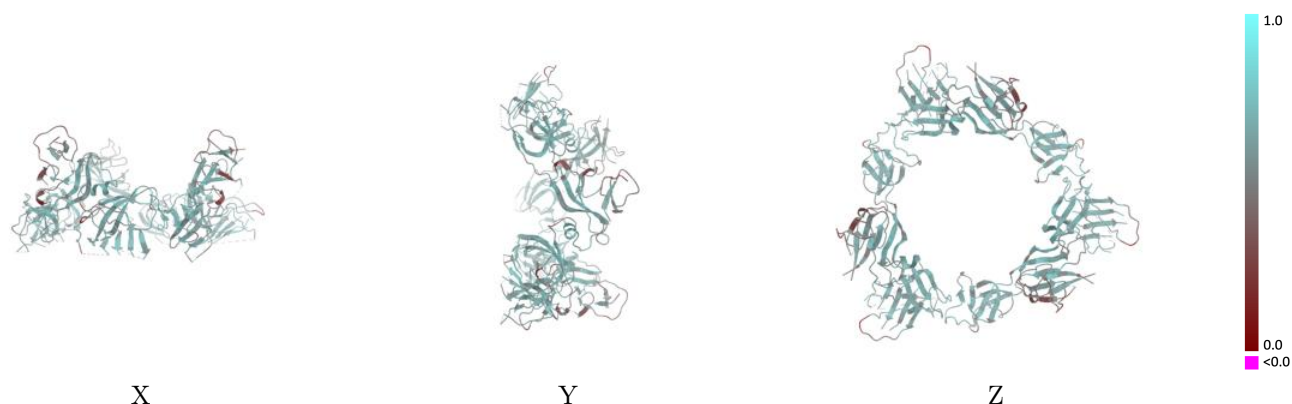
Y



Z

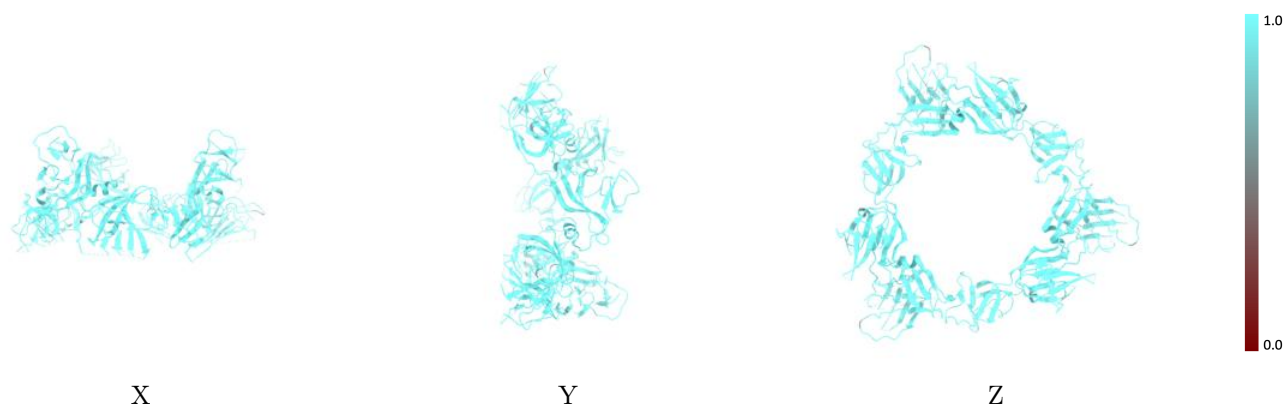
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



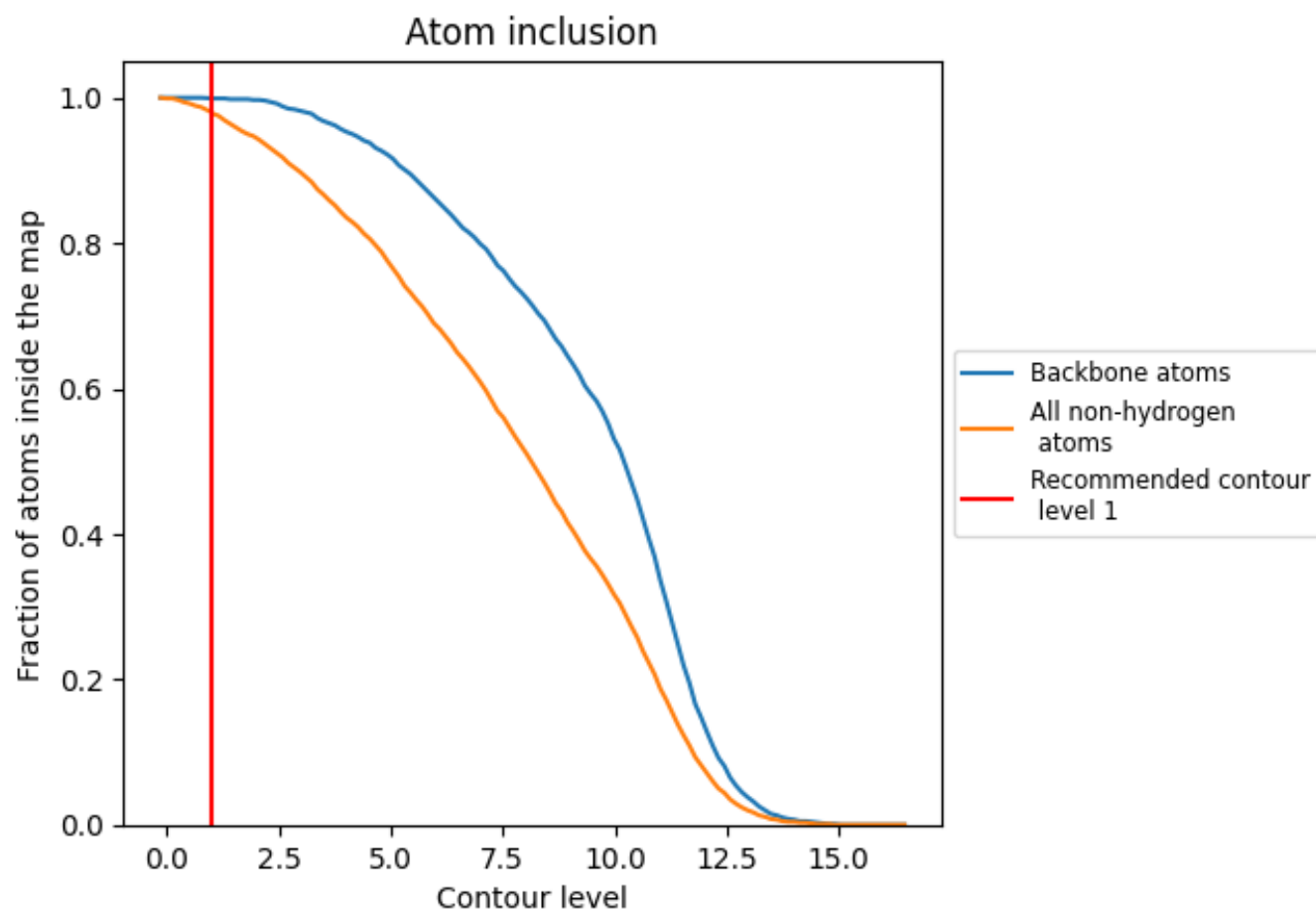
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9800	<div><div></div></div> 0.5600
A	<div><div></div></div> 0.9810	<div><div></div></div> 0.5610
B	<div><div></div></div> 0.9820	<div><div></div></div> 0.5620
C	<div><div></div></div> 0.9820	<div><div></div></div> 0.5600
D	<div><div></div></div> 0.8570	<div><div></div></div> 0.4420
E	<div><div></div></div> 0.8570	<div><div></div></div> 0.4430
F	<div><div></div></div> 0.8570	<div><div></div></div> 0.4390

1.0

0.0

<0.0