



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 09:26 PM EST

PDB ID : 7SIX
EMDB ID : EMD-25148
Title : Antibody N3-1 bound to RBDs in the up and down conformations
Authors : Hsieh, C.-L.; McLellan, J.S.
Deposited on : 2021-10-15
Resolution : 3.16 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

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>.

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

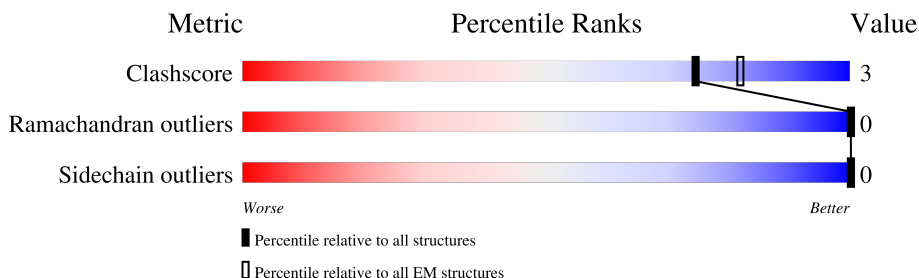
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	
2	H	128	
3	L	108	
4	C	2	
4	D	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4621 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	179	Total	C	N	O	S	0	0
			1437	928	239	265	5		
1	B	159	Total	C	N	O	S	0	0
			1282	825	215	238	4		

There are 178 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	1232	LEU	-	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	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	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
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
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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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	LEU	-	expression tag	UNP P0DTC2
B	1233	LEU	-	expression tag	UNP P0DTC2
B	1234	SER	-	expression tag	UNP P0DTC2
B	1235	THR	-	expression tag	UNP P0DTC2
B	1236	PHE	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	GLY	-	expression tag	UNP P0DTC2
B	1239	ARG	-	expression tag	UNP P0DTC2
B	1240	SER	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	VAL	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	PHE	-	expression tag	UNP P0DTC2
B	1246	GLN	-	expression tag	UNP P0DTC2
B	1247	GLY	-	expression tag	UNP P0DTC2
B	1248	PRO	-	expression tag	UNP P0DTC2
B	1249	GLY	-	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	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	ALA	-	expression tag	UNP P0DTC2
B	1260	TRP	-	expression tag	UNP P0DTC2
B	1261	SER	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1263	PRO	-	expression tag	UNP P0DTC2
B	1264	GLN	-	expression tag	UNP P0DTC2
B	1265	PHE	-	expression tag	UNP P0DTC2
B	1266	GLU	-	expression tag	UNP P0DTC2
B	1267	LYS	-	expression tag	UNP P0DTC2
B	1268	GLY	-	expression tag	UNP P0DTC2
B	1269	GLY	-	expression tag	UNP P0DTC2
B	1270	GLY	-	expression tag	UNP P0DTC2
B	1271	SER	-	expression tag	UNP P0DTC2
B	1272	GLY	-	expression tag	UNP P0DTC2
B	1273	GLY	-	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	GLY	-	expression tag	UNP P0DTC2
B	1278	GLY	-	expression tag	UNP P0DTC2
B	1279	SER	-	expression tag	UNP P0DTC2
B	1280	ALA	-	expression tag	UNP P0DTC2
B	1281	TRP	-	expression tag	UNP P0DTC2
B	1282	SER	-	expression tag	UNP P0DTC2
B	1283	HIS	-	expression tag	UNP P0DTC2
B	1284	PRO	-	expression tag	UNP P0DTC2
B	1285	GLN	-	expression tag	UNP P0DTC2
B	1286	PHE	-	expression tag	UNP P0DTC2
B	1287	GLU	-	expression tag	UNP P0DTC2
B	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called N3-1 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	128	Total	C	N	O	S	0	0
			1015	647	171	194	3		

- Molecule 3 is a protein called N3-1 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	108	Total	C	N	O	S	0	0
			831	525	135	168	3		

- 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	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

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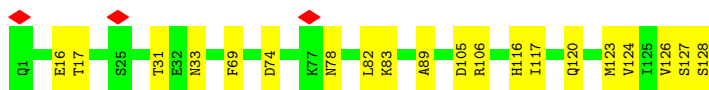
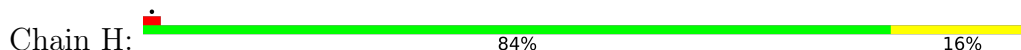
- Molecule 1: Spike glycoprotein



THR	THR	SER	THR	THR	VAL	C379	◆	CYS	LEU	GLY	ASN	ASN	MET
ILE	TYR	TYR	PRO	GLY	ASN	GLY	◆	THR	LEU	LYS	GLN	VAL	PHE
SER	GLU	GLU	THR	PHE	ASN	Y380	◆	LEU	ALA	GLY	THR	THR	LEU
VAL	CYS	ASP	ASN	PHE	ASN	VAL	◆	LYS	ASN	ASN	ASN	PHE	ASN
THR	ILE	ILE	THR	THR	ASN	SER	◆	THR	ARG	PHE	VAL	HIS	VAL
GLU	PRO	PRO	SER	GLY	GLY	THR	◆	PHE	SER	SER	VAL	ALA	LEU
ILE	ILE	ILE	ASN	GLN	LEU	THR	◆	VAL	TYR	ASN	ILE	ALA	LEU
PRO	ALA	ALA	GLN	THR	GLY	ASN	◆	LYS	THR	ARG	VAL	HIS	PRO
VAL	GLY	GLY	ALA	VAL	THR	ASP	◆	GLY	PRO	PHE	CYS	VAL	VAL
SER	ILE	ILE	VAL	VAL	GLY	ASP	◆	ILE	GLY	GLU	GLY	SER	SER
MET	CYS	CYS	LEU	LEU	VAL	LEU	◆	TYR	ASP	VAL	PHE	THR	SER
THR	ALA	ALA	TYR	GLN	LEU	CYS	◆	GLN	SER	PHE	GLN	ASN	CYS
LYS	SER	SER	GLN	THR	THR	PHE	◆	THR	SER	LYS	THR	THR	THR
THR	THR	GLU	ASP	VAL	GLU	THR	◆	SER	SER	ASN	THR	VAL	THR
VAL	THR	THR	ASN	ASN	LYS	V395	◆	PHE	THR	ILE	ASN	LYS	ASN
ASP	ASN	GLN	CYS	THR	LYS	D398	◆	ARG	THR	GLY	PRO	ARG	THR
CYS	THR	THR	THR	PHE	LYS	◆	◆	VAL	ALA	TYR	PHE	ASP	THR
THR	ASN	ASN	GLU	GLU	PHE	G413	◆	GLN	GLY	PHE	LEU	ARG	ARG
MET	SER	SER	VAL	LEU	LEU	◆	◆	THR	ALA	LYS	GLY	VAL	THR
TYR	PRO	PRO	PRO	PRO	PRO	D427	◆	THR	ALA	ILE	TYR	VAL	LEU
ILE	GLY	GLY	VAL	PHE	PHE	◆	◆	GLU	ALA	TYR	SER	TYR	LEU
CYS	SER	SER	ALA	GLN	GLN	◆	◆	SER	TYR	LYS	HIS	PRO	PRO
GLY	ALA	ALA	ILE	GLN	GLN	T430	◆	ILE	TYR	LYS	LYS	PHE	ALA
ASP	SER	SER	HIS	PHE	PHE	G431	◆	VAL	VAL	HIS	ASN	ASN	ALA
SER	SER	SER	ALA	GLY	ARG	G432	◆	ARG	GLY	THR	GLY	GLY	THR
THR	VAL	VAL	ASP	ASP	GLY	◆	◆	PHE	TYR	PRO	ASN	ASN	THR
GLU	ALA	ALA	GLN	ASP	ASP	◆	◆	PRO	LEU	ILE	LYS	VAL	THR
CYS	SER	SER	LEU	ILE	ILE	G446	◆	ASN	GLN	ASN	SER	TYR	SER
SER	GLN	GLN	THR	ALA	ALA	G447	◆	ILE	PRO	LEU	TPP	PHE	PHE
ASN	ASN	ASN	PRO	ASP	ASP	N448	◆	THR	ARG	VAL	MET	ALA	THR
LEU	ILE	ILE	THR	THR	THR	Y449	◆	ASN	THR	ARG	GLU	SER	ARG
LEU	ILE	ILE	TRP	THR	THR	N450	◆	LEU	PHE	ASP	SER	THR	GLY
LEU	LEU	ALA	ARG	ASP	ASP	◆	◆	CYS	LEU	LEU	GLU	THR	GLY
GLN	TYR	TYR	VAL	VAL	ALA	R466	◆	PRO	LEU	PRO	PHE	LYS	TYR
TYR	THR	THR	TYR	THR	VAL	◆	◆	F338	LYS	GLN	ARG	SER	TYR
GLY	MET	MET	SER	ARG	VAL	F515	◆	THR	TYR	GLY	ASN	THR	PRO
SER	SER	SER	THR	ASP	ASP	GLU	◆	ASN	ASN	PHE	TYR	VAL	ASN
PHE	LEU	LEU	GLY	PRO	PRO	LEU	◆	N353	GLU	SER	ILE	ILE	LYS
CYS	GLY	GLY	SER	GLN	GLN	LEU	◆	N354	ASN	SER	ILE	ARG	LYS
THR	ALA	ALA	ASN	THR	THR	HIS	◆	R355	GLY	LEU	ALA	GLY	PHE
GLN	GLU	GLU	VAL	VAL	THR	ALA	◆	K356	THR	THR	ASN	TRP	ARG
LEU	LEU	ASN	PHE	LEU	LEU	ALA	◆	R357	ILE	PRO	ASN	ILE	SER
ASN	SER	SER	GLN	ILE	ILE	PRO	◆	K358	THR	THR	CYS	PHE	SER
ARG	VAL	VAL	THR	LEU	LEU	ALA	◆	S359	ASP	VAL	THR	GLY	LEU
ALA	ALA	ALA	ALA	ASP	ASP	VAL	◆	ASN	ALA	ASP	PHE	THR	LEU
LEU	LEU	TYR	ALA	ILE	ILE	CYS	◆	CYS	VAL	LEU	GLU	THR	HIS
THR	SER	SER	GLY	THR	THR	GLY	◆	THR	ASP	PRO	TYR	LEU	SER
GLY	ASN	ASN	CYS	PRO	PRO	GLY	◆	VAL	CYS	ILE	VAL	ASP	THR
ILE	ASN	ASN	LEU	SER	SER	VAL	◆	ALA	ALA	GLY	THR	THR	GLN
ALA	SER	SER	LEU	ILE	ILE	LYS	◆	THR	LEU	ILE	GLN	LYS	ASN
VAL	VAL	ILE	GLY	PHE	PHE	SER	◆	S366	ASP	ILE	PHE	THR	THR
GLU	GLU	ALA	ALA	GLY	GLY	THR	◆	ASN	VAL	THR	LEU	SER	LEU
GLN	ILE	ILE	GLU	GLY	GLY	ASN	◆	Y369	LEU	THR	GLN	GLN	PHE
ASP	PRO	PRO	HIS	VAL	VAL	ASN	◆	K370	SER	ARG	MET	LEU	LEU
LYS	THR	THR	VAL	VAL	VAL	S371	◆	S371	GLU	PHE	ASP	LEU	PHE
THR	ASN	PHE	ASN	ILE	ILE	ASN	◆	THR	LYS	THR	GLU	VAL	SER

[illegible]

- Molecule 2: N3-1 Fab heavy chain



- Molecule 3: N3-1 Fab light chain



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



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



MAG
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	269553	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.203	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.34	Depositor
Map size (\AA)	475.2, 475.2, 475.2	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	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	0.27	0/1479	0.49	0/2009
1	B	0.29	0/1317	0.50	0/1784
2	H	0.28	0/1046	0.53	0/1427
3	L	0.27	0/852	0.52	0/1159
All	All	0.28	0/4694	0.51	0/6379

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	1437	0	1361	11	0
1	B	1282	0	1207	6	0
2	H	1015	0	954	12	0
3	L	831	0	796	1	0
4	C	28	0	25	0	0
4	D	28	0	25	0	0
All	All	4621	0	4368	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (29) 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:357:ARG:NH2	1:A:393:THR:O	2.26	0.69
1:A:406:GLU:OE1	1:A:409:GLN:NE2	2.30	0.64
1:A:357:ARG:NH1	1:A:358:ILE:O	2.31	0.64
2:H:105:ASP:OD1	2:H:106:ARG:N	2.32	0.62
2:H:16:GLU:HG3	2:H:17:THR:H	1.66	0.61
2:H:31:THR:HG22	2:H:33:ASN:H	1.66	0.60
2:H:89:ALA:HA	2:H:126:VAL:HG21	1.84	0.59
2:H:74:ASP:O	2:H:78:ASN:N	2.36	0.58
1:B:446:GLY:O	2:H:83:LYS:NZ	2.32	0.57
1:B:448:ASN:OD1	1:B:450:ASN:ND2	2.36	0.56
1:A:457:ARG:NH1	1:A:459:SER:O	2.39	0.53
2:H:123:MET:SD	2:H:124:VAL:N	2.83	0.52
1:B:395:VAL:HG12	1:B:515:PHE:CD1	2.46	0.50
1:A:476:GLY:N	1:A:487:ASN:OD1	2.44	0.49
1:B:355:ARG:NH2	1:B:398:ASP:OD1	2.45	0.49
2:H:116:HIS:O	2:H:117:ILE:HD13	2.14	0.47
2:H:16:GLU:HG3	2:H:17:THR:N	2.29	0.46
1:A:462:LYS:N	1:A:465:GLU:OE2	2.38	0.46
1:A:462:LYS:HA	1:A:462:LYS:HE2	1.99	0.45
2:H:69:PHE:HD2	2:H:82:LEU:HD21	1.80	0.44
1:A:357:ARG:NH2	1:A:394:ASN:HA	2.33	0.44
3:L:55:GLU:O	3:L:58:VAL:HG22	2.17	0.44
1:A:468:ILE:HG13	1:A:469:SER:N	2.34	0.42
1:B:353:TRP:O	1:B:466:ARG:NH1	2.48	0.42
1:A:473:TYR:HB3	1:A:489:TYR:O	2.21	0.41
2:H:120:GLN:HA	2:H:120:GLN:OE1	2.20	0.41
2:H:127:SER:OG	2:H:128:SER:N	2.53	0.41
1:B:370:ASN:OD1	1:B:371:SER:N	2.54	0.41
1:A:408:ARG:NH1	1:A:414:GLN:HE22	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	175/1288 (14%)	170 (97%)	5 (3%)	0	100	100
1	B	153/1288 (12%)	147 (96%)	6 (4%)	0	100	100
2	H	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
3	L	106/108 (98%)	101 (95%)	5 (5%)	0	100	100
All	All	560/2812 (20%)	537 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	154/1116 (14%)	154 (100%)	0	100	100
1	B	137/1116 (12%)	137 (100%)	0	100	100
2	H	111/111 (100%)	111 (100%)	0	100	100
3	L	93/94 (99%)	93 (100%)	0	100	100
All	All	495/2437 (20%)	495 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	501	ASN
2	H	5	GLN

5.3.3 RNA ⓘ

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](#)

4 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	C	1	4,1	14,14,15	0.23	0	17,19,21	0.39	0
4	NAG	C	2	4	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	D	1	4,1	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	D	2	4	14,14,15	0.22	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
4	NAG	C	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	NAG	O5-C5-C6-O6
4	C	2	NAG	O5-C5-C6-O6

Continued on next page...

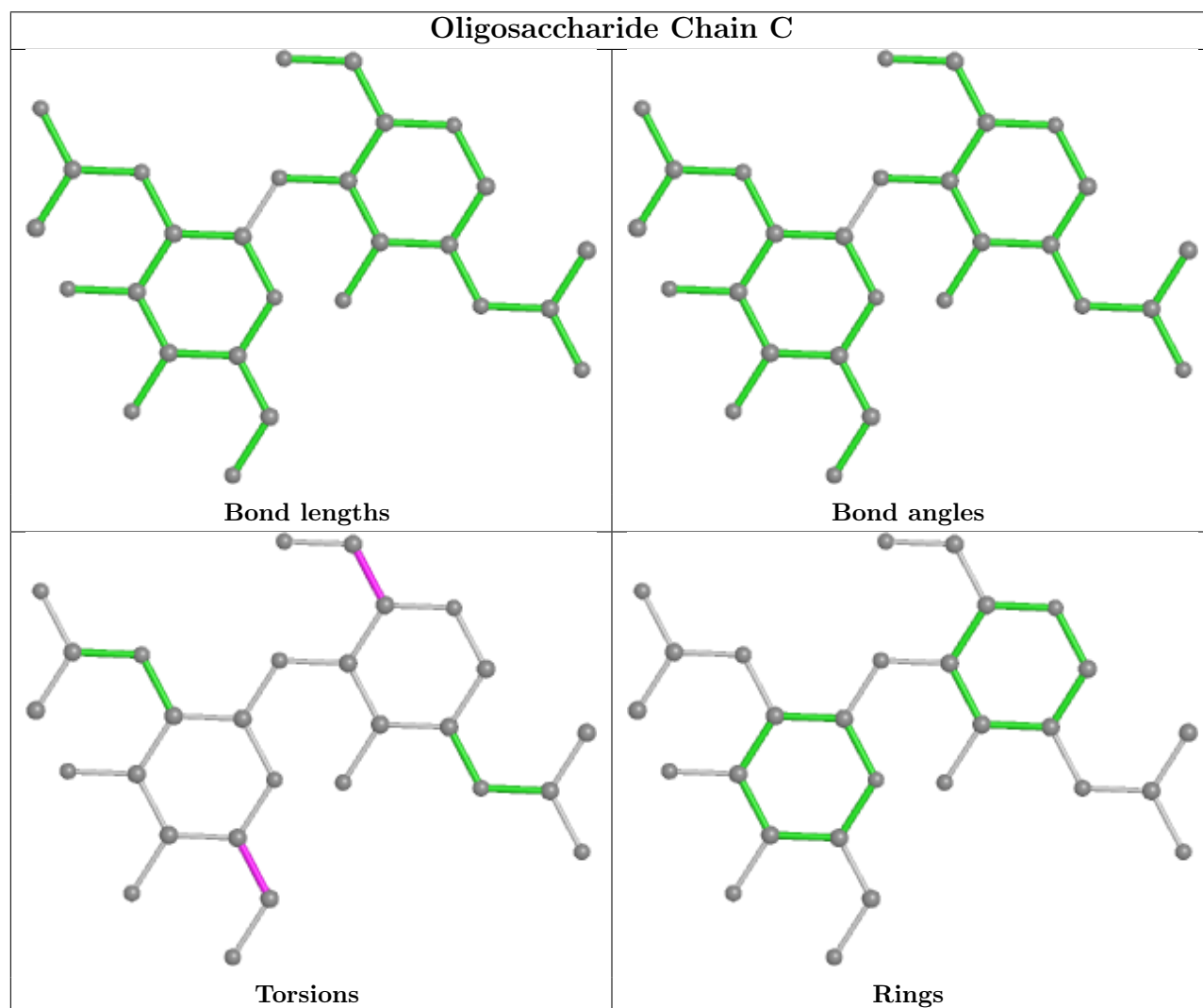
Continued from previous page...

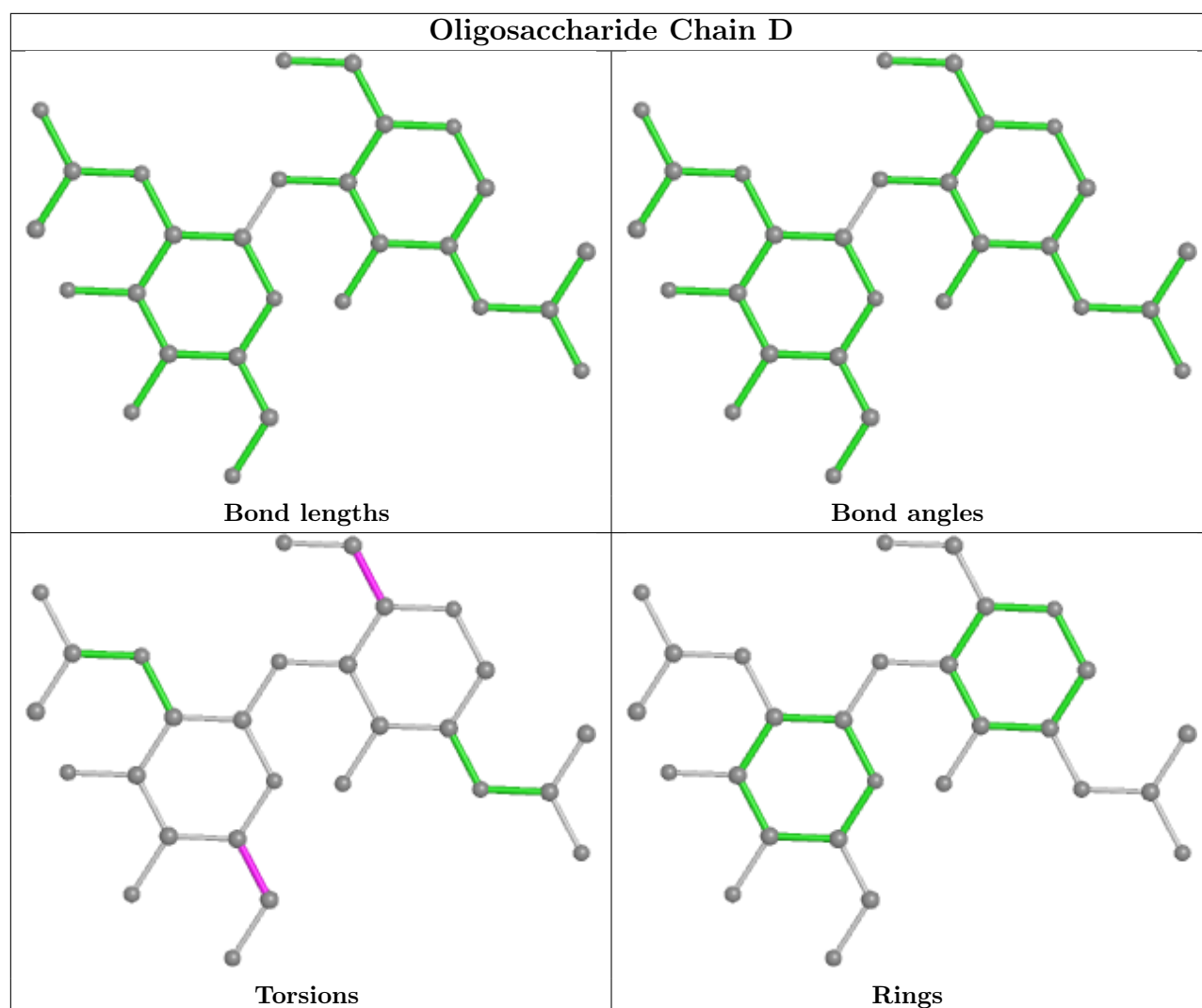
Mol	Chain	Res	Type	Atoms
4	C	1	NAG	C4-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6

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](#)

There are no ligands in this entry.

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.

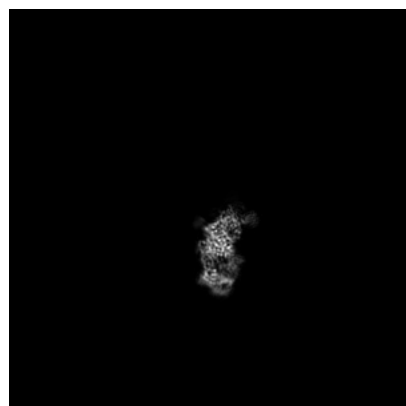
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25148. These allow visual inspection of the internal detail of the map and identification of artifacts.

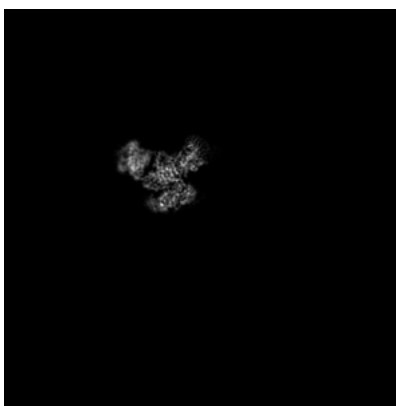
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

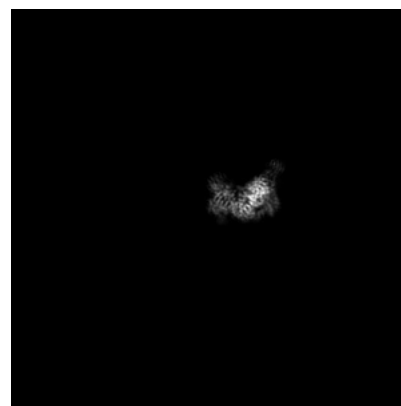
6.1.1 Primary map



X

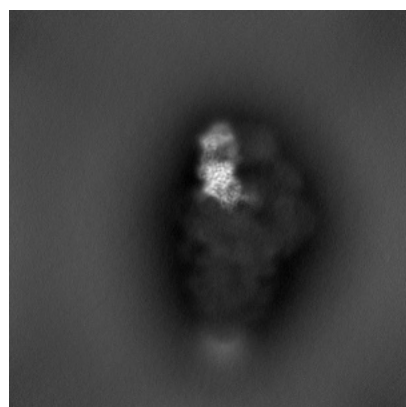


Y

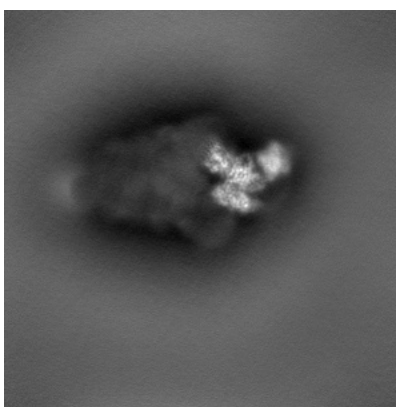


Z

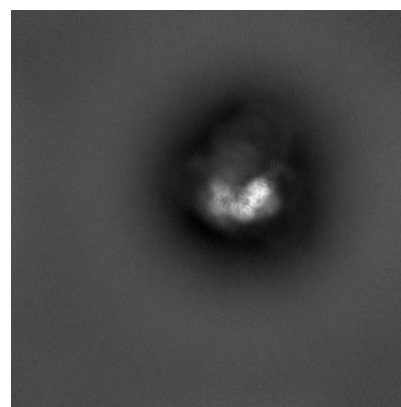
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

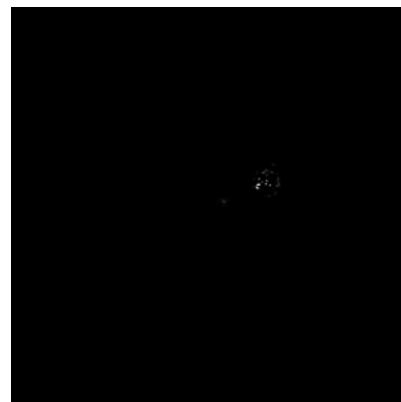
6.2.1 Primary map



X Index: 216

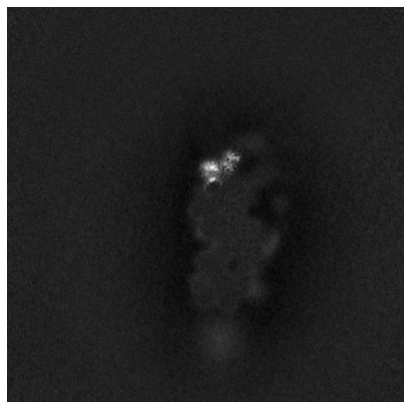


Y Index: 216

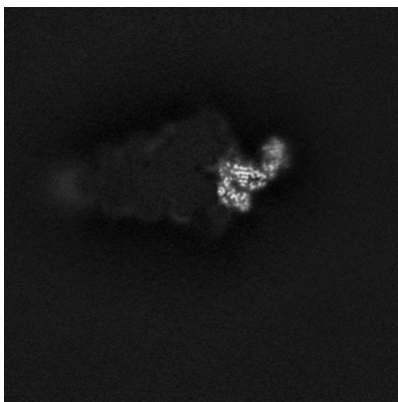


Z Index: 216

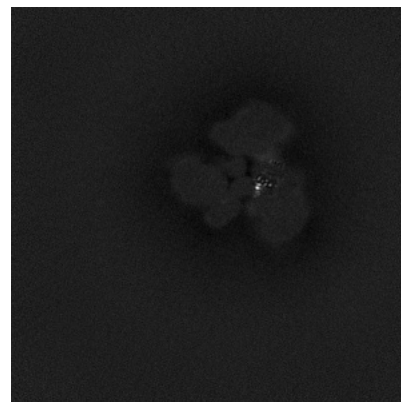
6.2.2 Raw map



X Index: 216



Y Index: 216



Z Index: 216

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

6.3 Largest variance slices [i](#)

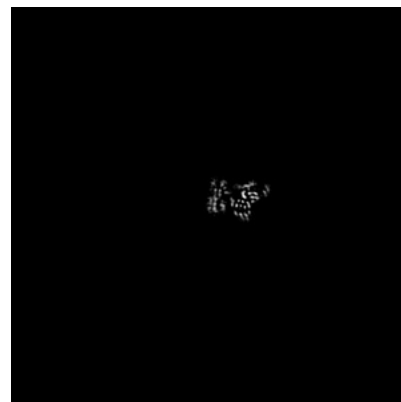
6.3.1 Primary map



X Index: 261

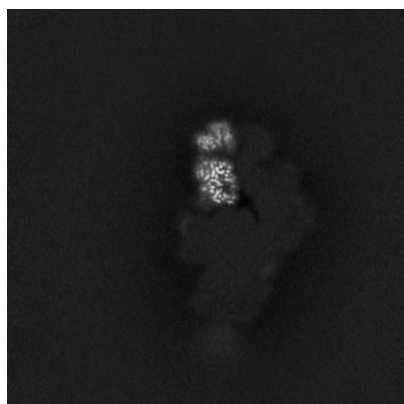


Y Index: 229

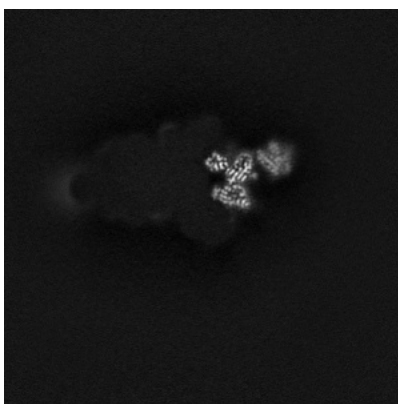


Z Index: 171

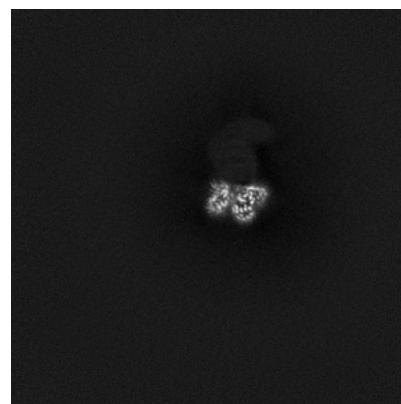
6.3.2 Raw map



X Index: 259



Y Index: 230

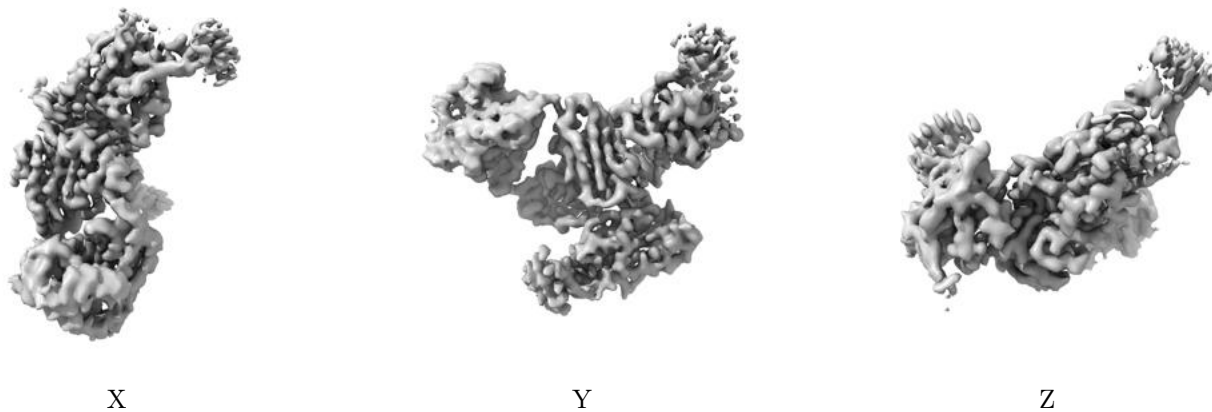


Z Index: 256

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

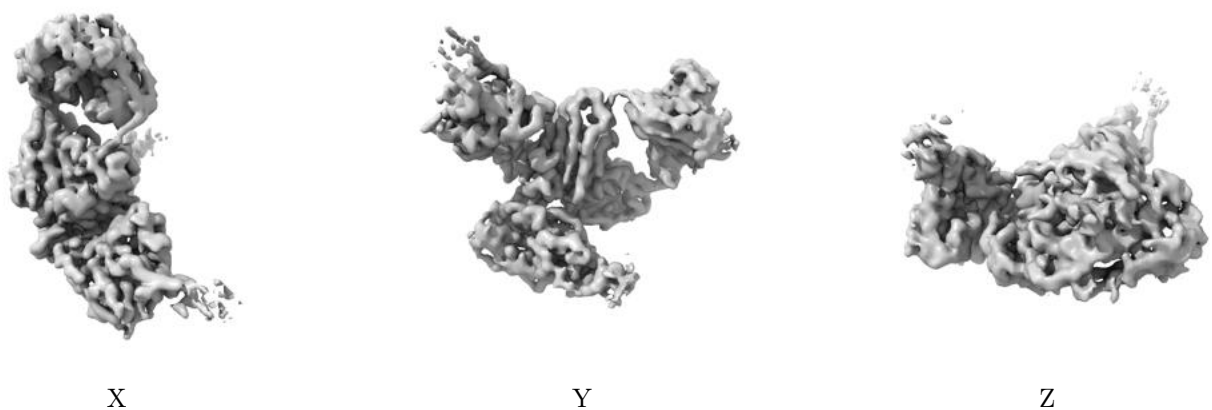
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.34. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

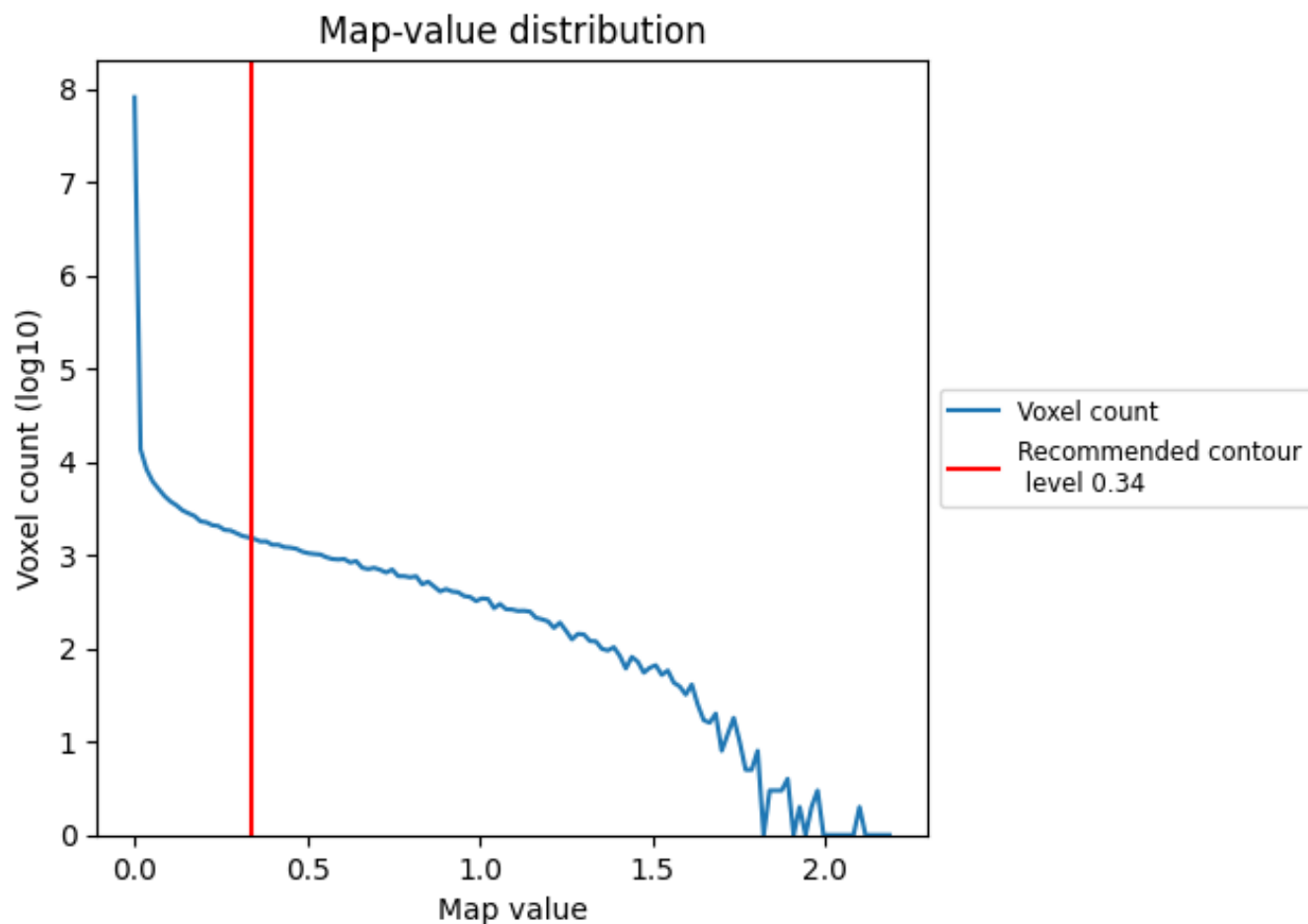
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

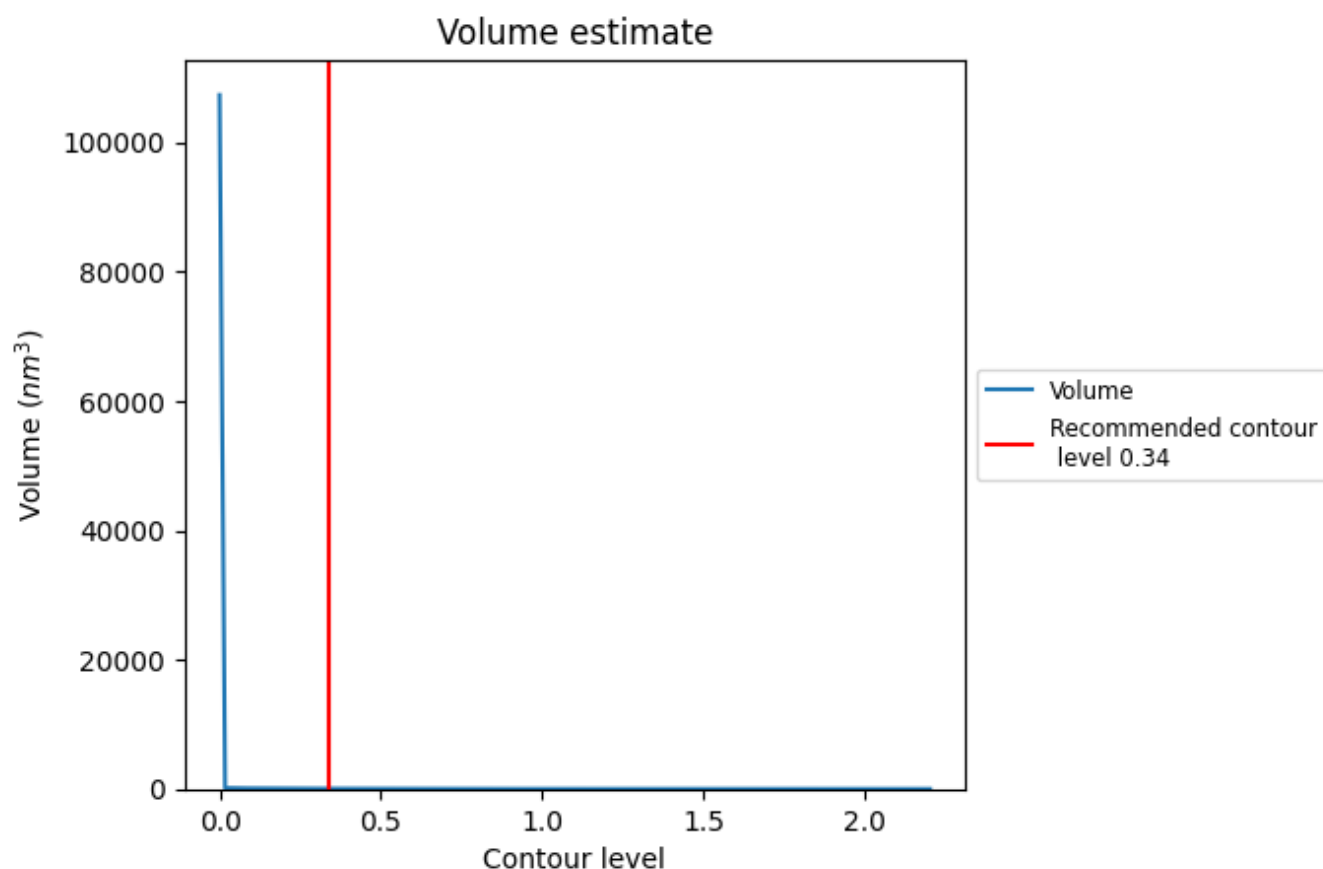
This section contains the results of statistical analysis of the map.

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.

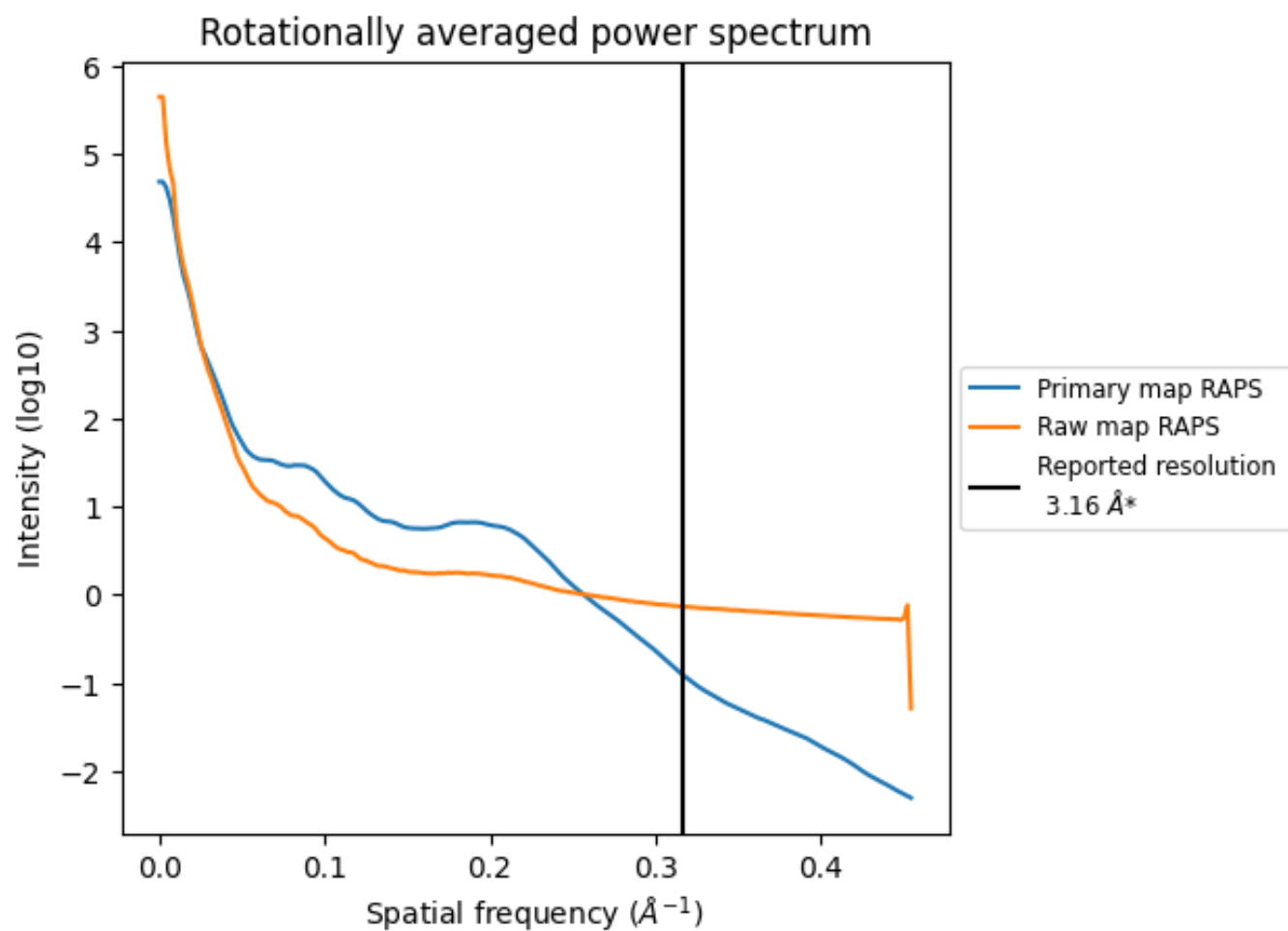
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49 nm^3 ; this corresponds to an approximate mass of 44 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 ⓘ

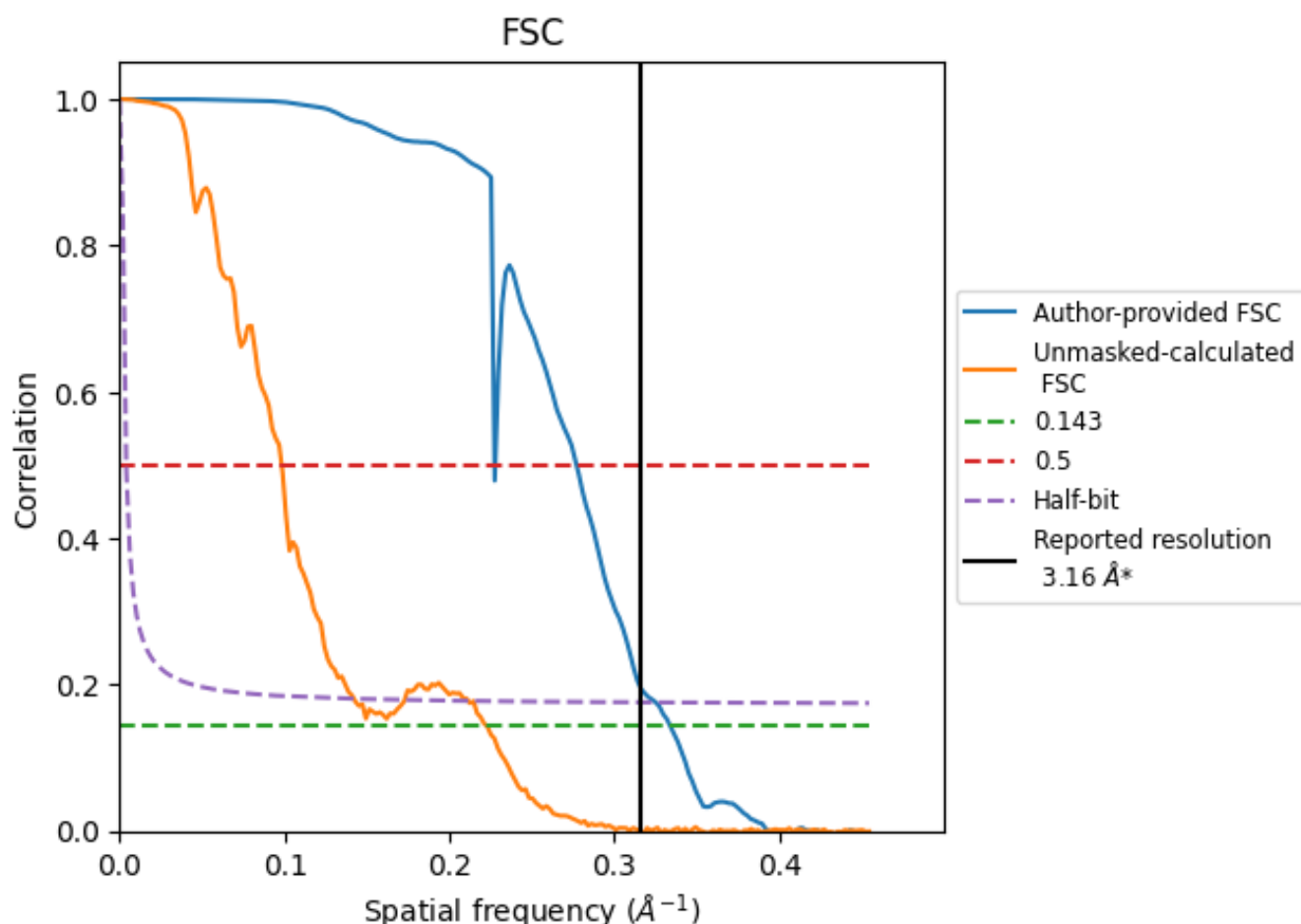


*Reported resolution corresponds to spatial frequency of 0.316 \AA^{-1}

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 0.316 Å⁻¹

8.2 Resolution estimates [i](#)

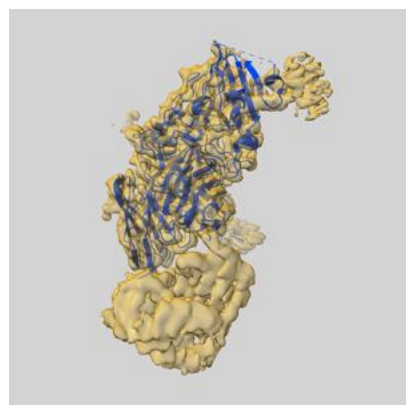
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	2.99	4.40	3.08
Unmasked-calculated*	4.49	10.17	7.04

*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 4.49 differs from the reported value 3.16 by more than 10 %

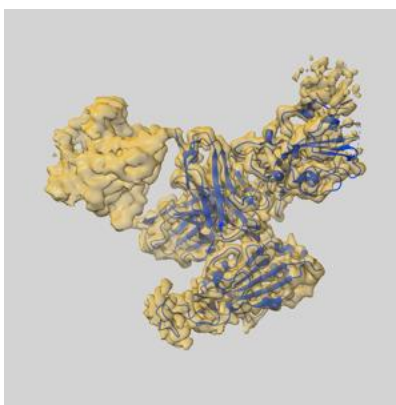
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25148 and PDB model 7SIX. Per-residue inclusion information can be found in section 3 on page 9.

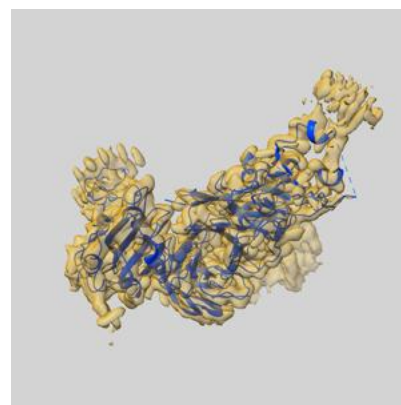
9.1 Map-model overlay [i](#)



X



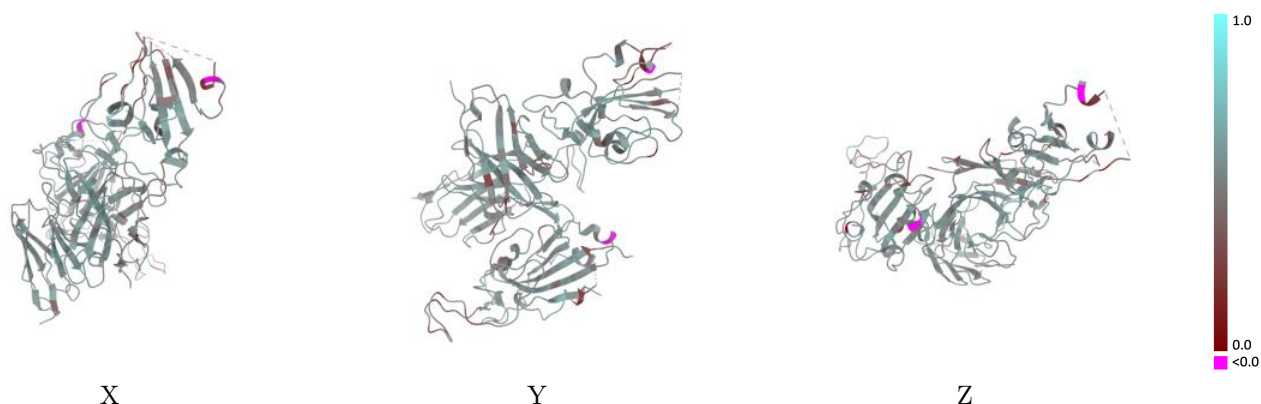
Y



Z

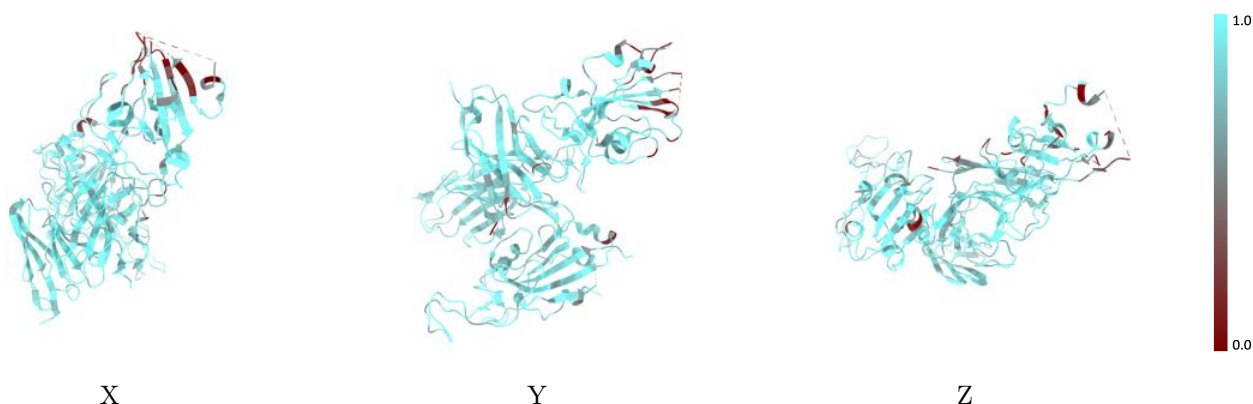
The images above show the 3D surface view of the map at the recommended contour level 0.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



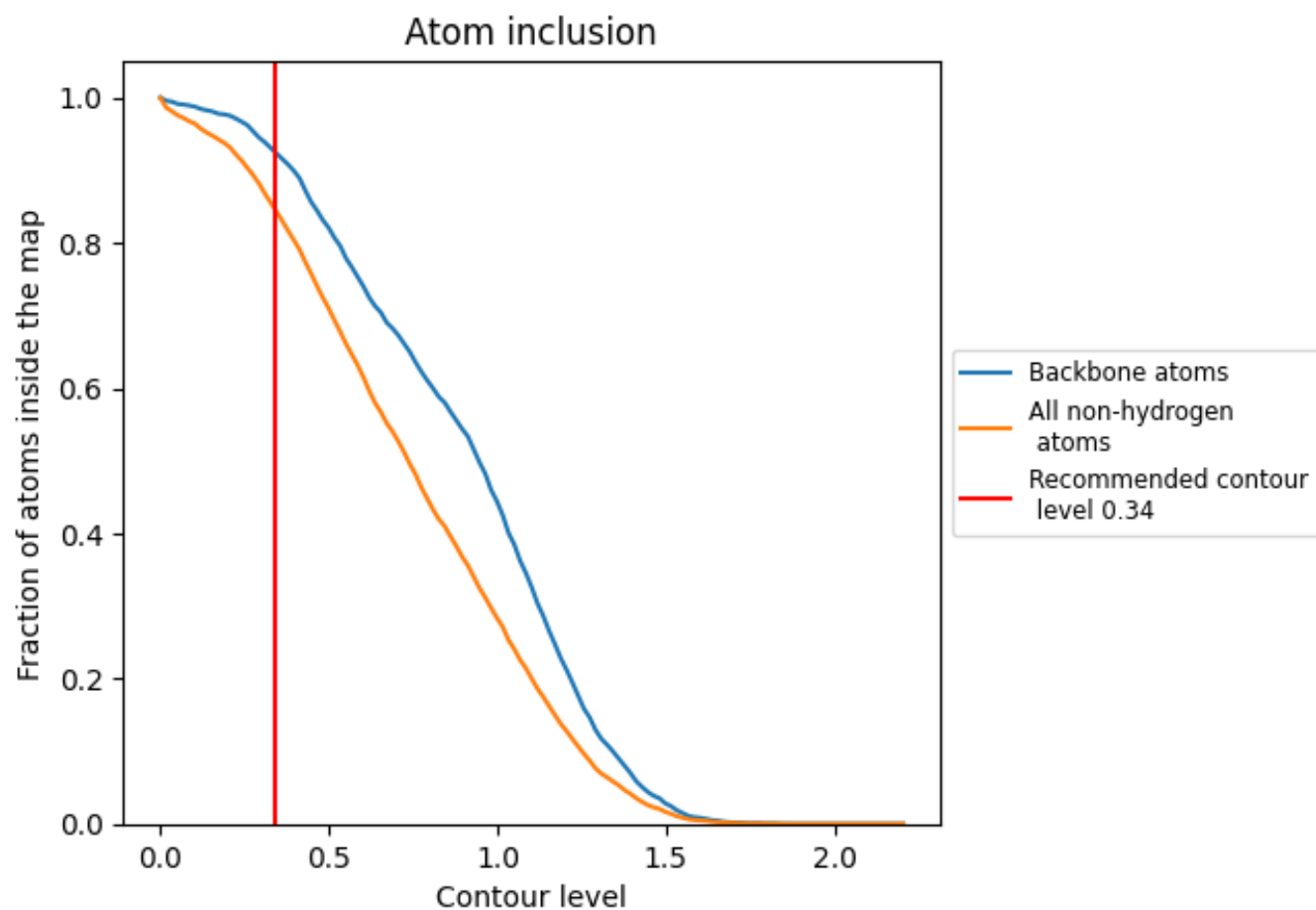
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.34).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 85% 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 (0.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8457	<div><div></div></div> 0.5070
A	<div><div></div></div> 0.8502	<div><div></div></div> 0.4910
B	<div><div></div></div> 0.8053	<div><div></div></div> 0.5100
C	<div><div></div></div> 0.8214	<div><div></div></div> 0.5200
D	<div><div></div></div> 0.7143	<div><div></div></div> 0.3380
H	<div><div></div></div> 0.8586	<div><div></div></div> 0.5160
L	<div><div></div></div> 0.8897	<div><div></div></div> 0.5270

1.0

0.0

<0.0