



## wwPDB EM Validation Summary Report ⓘ

Sep 12, 2024 – 04:14 PM EDT

PDB ID : 9ATP  
EMDB ID : EMD-43832  
Title : local refinement of XBB.1.5 spike/Nanosota-3C complex  
Authors : Ye, G.; Bu, F.; Liu, B.; Li, F.  
Deposited on : 2024-02-27  
Resolution : 3.50 Å(reported)  
Based on initial model : 8vkl

This is a wwPDB EM Validation Summary 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.dev112  
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) : 2.38.3

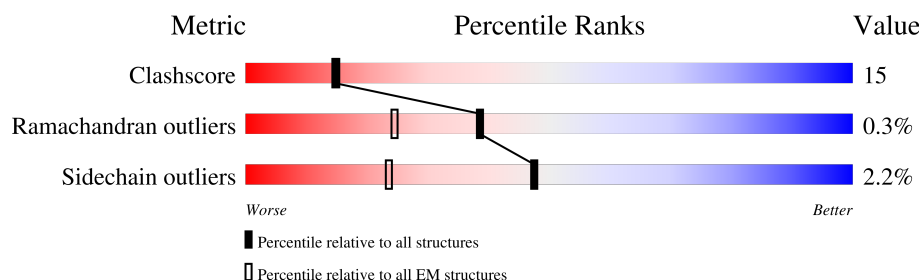
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*







The reported resolution of this entry is 3.50 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	1230	
1	B	1230	
1	C	1230	
2	D	136	
2	E	136	
2	L	136	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13004 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	438	Total	C	N	O	S	0	0
			3513	2278	575	646	14		
1	B	436	Total	C	N	O	S	0	0
			3498	2267	573	644	14		
1	C	417	Total	C	N	O	S	0	0
			3356	2181	546	617	12		

There are 255 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	24	SER	ALA	variant	UNP P0DTC2
A	80	ALA	VAL	variant	UNP P0DTC2
A	139	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	142	GLN	HIS	variant	UNP P0DTC2
A	179	GLU	GLN	variant	UNP P0DTC2
A	209	GLU	VAL	variant	UNP P0DTC2
A	335	HIS	GLY	variant	UNP P0DTC2
A	342	THR	ARG	variant	UNP P0DTC2
A	364	ILE	LEU	variant	UNP P0DTC2
A	367	PHE	SER	variant	UNP P0DTC2
A	369	PRO	SER	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	372	ALA	THR	variant	UNP P0DTC2
A	401	ASN	ASP	variant	UNP P0DTC2
A	404	SER	ARG	variant	UNP P0DTC2
A	413	ASN	LYS	variant	UNP P0DTC2
A	436	LYS	ASN	variant	UNP P0DTC2
A	441	PRO	VAL	variant	UNP P0DTC2
A	442	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	456	LYS	ASN	variant	UNP P0DTC2
A	473	ASN	SER	variant	UNP P0DTC2
A	474	LYS	THR	variant	UNP P0DTC2
A	480	ALA	GLU	variant	UNP P0DTC2
A	482	PRO	PHE	variant	UNP P0DTC2
A	486	SER	PHE	variant	UNP P0DTC2
A	494	ARG	GLN	variant	UNP P0DTC2
A	497	TYR	ASN	variant	UNP P0DTC2
A	501	HIS	TYR	variant	UNP P0DTC2
A	610	GLY	ASP	variant	UNP P0DTC2
A	651	TYR	HIS	variant	UNP P0DTC2
A	675	LYS	ASN	variant	UNP P0DTC2
A	677	HIS	PRO	variant	UNP P0DTC2
A	678	ALA	ARG	engineered mutation	UNP P0DTC2
A	679	GLY	ARG	engineered mutation	UNP P0DTC2
A	760	LYS	ASN	variant	UNP P0DTC2
A	792	TYR	ASP	variant	UNP P0DTC2
A	813	PRO	PHE	engineered mutation	UNP P0DTC2
A	888	PRO	ALA	engineered mutation	UNP P0DTC2
A	895	PRO	ALA	engineered mutation	UNP P0DTC2
A	938	PRO	ALA	engineered mutation	UNP P0DTC2
A	950	HIS	GLN	variant	UNP P0DTC2
A	965	LYS	ASN	variant	UNP P0DTC2
A	982	PRO	LYS	engineered mutation	UNP P0DTC2
A	983	PRO	VAL	engineered mutation	UNP P0DTC2
A	1208	GLY	-	expression tag	UNP P0DTC2
A	1209	SER	-	expression tag	UNP P0DTC2
A	1210	GLY	-	expression tag	UNP P0DTC2
A	1211	TYR	-	expression tag	UNP P0DTC2
A	1212	ILE	-	expression tag	UNP P0DTC2
A	1213	PRO	-	expression tag	UNP P0DTC2
A	1214	GLU	-	expression tag	UNP P0DTC2
A	1215	ALA	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	ARG	-	expression tag	UNP P0DTC2
A	1218	ASP	-	expression tag	UNP P0DTC2
A	1219	GLY	-	expression tag	UNP P0DTC2
A	1220	GLN	-	expression tag	UNP P0DTC2
A	1221	ALA	-	expression tag	UNP P0DTC2
A	1222	TYR	-	expression tag	UNP P0DTC2
A	1223	VAL	-	expression tag	UNP P0DTC2
A	1224	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1225	LYS	-	expression tag	UNP P0DTC2
A	1226	ASP	-	expression tag	UNP P0DTC2
A	1227	GLY	-	expression tag	UNP P0DTC2
A	1228	GLU	-	expression tag	UNP P0DTC2
A	1229	TRP	-	expression tag	UNP P0DTC2
A	1230	VAL	-	expression tag	UNP P0DTC2
A	1231	LEU	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	SER	-	expression tag	UNP P0DTC2
A	1234	THR	-	expression tag	UNP P0DTC2
A	1235	PHE	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	GLY	-	expression tag	UNP P0DTC2
A	1238	HIS	-	expression tag	UNP P0DTC2
A	1239	HIS	-	expression tag	UNP P0DTC2
A	1240	HIS	-	expression tag	UNP P0DTC2
A	1241	HIS	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	24	SER	ALA	variant	UNP P0DTC2
B	80	ALA	VAL	variant	UNP P0DTC2
B	139	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	142	GLN	HIS	variant	UNP P0DTC2
B	179	GLU	GLN	variant	UNP P0DTC2
B	209	GLU	VAL	variant	UNP P0DTC2
B	335	HIS	GLY	variant	UNP P0DTC2
B	342	THR	ARG	variant	UNP P0DTC2
B	364	ILE	LEU	variant	UNP P0DTC2
B	367	PHE	SER	variant	UNP P0DTC2
B	369	PRO	SER	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	372	ALA	THR	variant	UNP P0DTC2
B	401	ASN	ASP	variant	UNP P0DTC2
B	404	SER	ARG	variant	UNP P0DTC2
B	413	ASN	LYS	variant	UNP P0DTC2
B	436	LYS	ASN	variant	UNP P0DTC2
B	441	PRO	VAL	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	442	SER	GLY	variant	UNP P0DTC2
B	456	LYS	ASN	variant	UNP P0DTC2
B	473	ASN	SER	variant	UNP P0DTC2
B	474	LYS	THR	variant	UNP P0DTC2
B	480	ALA	GLU	variant	UNP P0DTC2
B	482	PRO	PHE	variant	UNP P0DTC2
B	486	SER	PHE	variant	UNP P0DTC2
B	494	ARG	GLN	variant	UNP P0DTC2
B	497	TYR	ASN	variant	UNP P0DTC2
B	501	HIS	TYR	variant	UNP P0DTC2
B	610	GLY	ASP	variant	UNP P0DTC2
B	651	TYR	HIS	variant	UNP P0DTC2
B	675	LYS	ASN	variant	UNP P0DTC2
B	677	HIS	PRO	variant	UNP P0DTC2
B	678	ALA	ARG	engineered mutation	UNP P0DTC2
B	679	GLY	ARG	engineered mutation	UNP P0DTC2
B	760	LYS	ASN	variant	UNP P0DTC2
B	792	TYR	ASP	variant	UNP P0DTC2
B	813	PRO	PHE	engineered mutation	UNP P0DTC2
B	888	PRO	ALA	engineered mutation	UNP P0DTC2
B	895	PRO	ALA	engineered mutation	UNP P0DTC2
B	938	PRO	ALA	engineered mutation	UNP P0DTC2
B	950	HIS	GLN	variant	UNP P0DTC2
B	965	LYS	ASN	variant	UNP P0DTC2
B	982	PRO	LYS	engineered mutation	UNP P0DTC2
B	983	PRO	VAL	engineered mutation	UNP P0DTC2
B	1208	GLY	-	expression tag	UNP P0DTC2
B	1209	SER	-	expression tag	UNP P0DTC2
B	1210	GLY	-	expression tag	UNP P0DTC2
B	1211	TYR	-	expression tag	UNP P0DTC2
B	1212	ILE	-	expression tag	UNP P0DTC2
B	1213	PRO	-	expression tag	UNP P0DTC2
B	1214	GLU	-	expression tag	UNP P0DTC2
B	1215	ALA	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	ARG	-	expression tag	UNP P0DTC2
B	1218	ASP	-	expression tag	UNP P0DTC2
B	1219	GLY	-	expression tag	UNP P0DTC2
B	1220	GLN	-	expression tag	UNP P0DTC2
B	1221	ALA	-	expression tag	UNP P0DTC2
B	1222	TYR	-	expression tag	UNP P0DTC2
B	1223	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1224	ARG	-	expression tag	UNP P0DTC2
B	1225	LYS	-	expression tag	UNP P0DTC2
B	1226	ASP	-	expression tag	UNP P0DTC2
B	1227	GLY	-	expression tag	UNP P0DTC2
B	1228	GLU	-	expression tag	UNP P0DTC2
B	1229	TRP	-	expression tag	UNP P0DTC2
B	1230	VAL	-	expression tag	UNP P0DTC2
B	1231	LEU	-	expression tag	UNP P0DTC2
B	1232	LEU	-	expression tag	UNP P0DTC2
B	1233	SER	-	expression tag	UNP P0DTC2
B	1234	THR	-	expression tag	UNP P0DTC2
B	1235	PHE	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	GLY	-	expression tag	UNP P0DTC2
B	1238	HIS	-	expression tag	UNP P0DTC2
B	1239	HIS	-	expression tag	UNP P0DTC2
B	1240	HIS	-	expression tag	UNP P0DTC2
B	1241	HIS	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	24	SER	ALA	variant	UNP P0DTC2
C	80	ALA	VAL	variant	UNP P0DTC2
C	139	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	142	GLN	HIS	variant	UNP P0DTC2
C	179	GLU	GLN	variant	UNP P0DTC2
C	209	GLU	VAL	variant	UNP P0DTC2
C	335	HIS	GLY	variant	UNP P0DTC2
C	342	THR	ARG	variant	UNP P0DTC2
C	364	ILE	LEU	variant	UNP P0DTC2
C	367	PHE	SER	variant	UNP P0DTC2
C	369	PRO	SER	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	372	ALA	THR	variant	UNP P0DTC2
C	401	ASN	ASP	variant	UNP P0DTC2
C	404	SER	ARG	variant	UNP P0DTC2
C	413	ASN	LYS	variant	UNP P0DTC2
C	436	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	441	PRO	VAL	variant	UNP P0DTC2
C	442	SER	GLY	variant	UNP P0DTC2
C	456	LYS	ASN	variant	UNP P0DTC2
C	473	ASN	SER	variant	UNP P0DTC2
C	474	LYS	THR	variant	UNP P0DTC2
C	480	ALA	GLU	variant	UNP P0DTC2
C	482	PRO	PHE	variant	UNP P0DTC2
C	486	SER	PHE	variant	UNP P0DTC2
C	494	ARG	GLN	variant	UNP P0DTC2
C	497	TYR	ASN	variant	UNP P0DTC2
C	501	HIS	TYR	variant	UNP P0DTC2
C	610	GLY	ASP	variant	UNP P0DTC2
C	651	TYR	HIS	variant	UNP P0DTC2
C	675	LYS	ASN	variant	UNP P0DTC2
C	677	HIS	PRO	variant	UNP P0DTC2
C	678	ALA	ARG	engineered mutation	UNP P0DTC2
C	679	GLY	ARG	engineered mutation	UNP P0DTC2
C	760	LYS	ASN	variant	UNP P0DTC2
C	792	TYR	ASP	variant	UNP P0DTC2
C	813	PRO	PHE	engineered mutation	UNP P0DTC2
C	888	PRO	ALA	engineered mutation	UNP P0DTC2
C	895	PRO	ALA	engineered mutation	UNP P0DTC2
C	938	PRO	ALA	engineered mutation	UNP P0DTC2
C	950	HIS	GLN	variant	UNP P0DTC2
C	965	LYS	ASN	variant	UNP P0DTC2
C	982	PRO	LYS	engineered mutation	UNP P0DTC2
C	983	PRO	VAL	engineered mutation	UNP P0DTC2
C	1208	GLY	-	expression tag	UNP P0DTC2
C	1209	SER	-	expression tag	UNP P0DTC2
C	1210	GLY	-	expression tag	UNP P0DTC2
C	1211	TYR	-	expression tag	UNP P0DTC2
C	1212	ILE	-	expression tag	UNP P0DTC2
C	1213	PRO	-	expression tag	UNP P0DTC2
C	1214	GLU	-	expression tag	UNP P0DTC2
C	1215	ALA	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	ARG	-	expression tag	UNP P0DTC2
C	1218	ASP	-	expression tag	UNP P0DTC2
C	1219	GLY	-	expression tag	UNP P0DTC2
C	1220	GLN	-	expression tag	UNP P0DTC2
C	1221	ALA	-	expression tag	UNP P0DTC2
C	1222	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1223	VAL	-	expression tag	UNP P0DTC2
C	1224	ARG	-	expression tag	UNP P0DTC2
C	1225	LYS	-	expression tag	UNP P0DTC2
C	1226	ASP	-	expression tag	UNP P0DTC2
C	1227	GLY	-	expression tag	UNP P0DTC2
C	1228	GLU	-	expression tag	UNP P0DTC2
C	1229	TRP	-	expression tag	UNP P0DTC2
C	1230	VAL	-	expression tag	UNP P0DTC2
C	1231	LEU	-	expression tag	UNP P0DTC2
C	1232	LEU	-	expression tag	UNP P0DTC2
C	1233	SER	-	expression tag	UNP P0DTC2
C	1234	THR	-	expression tag	UNP P0DTC2
C	1235	PHE	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	GLY	-	expression tag	UNP P0DTC2
C	1238	HIS	-	expression tag	UNP P0DTC2
C	1239	HIS	-	expression tag	UNP P0DTC2
C	1240	HIS	-	expression tag	UNP P0DTC2
C	1241	HIS	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Nanosota-3C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	115	Total	C	N	O	S	0	0
			879	551	153	171	4		
2	E	115	Total	C	N	O	S	0	0
			879	551	153	171	4		
2	L	115	Total	C	N	O	S	0	0
			879	551	153	171	4		



[illegible]

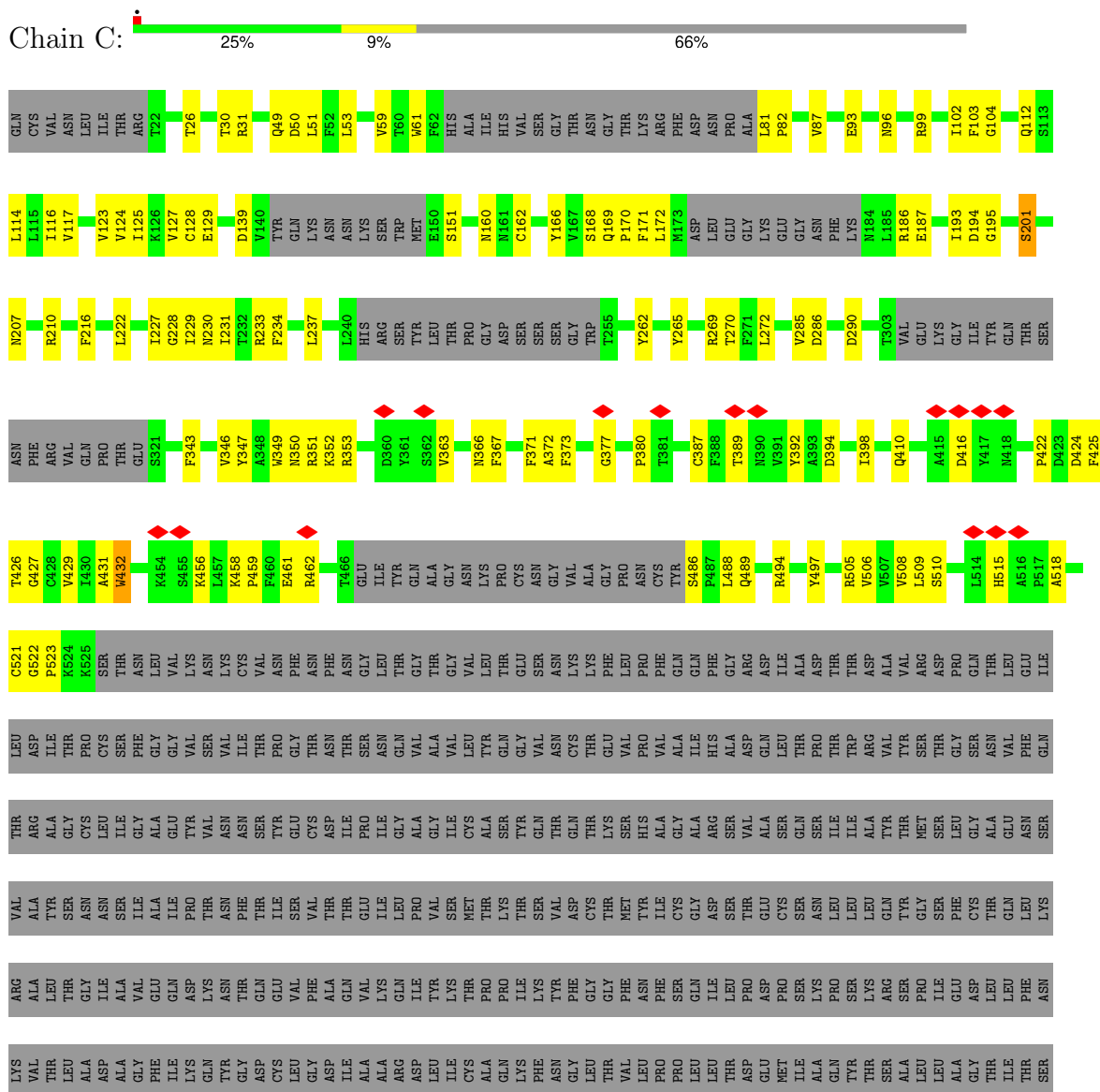
- Molecule 1: Spike glycoprotein

Chain B:  23% 12% 65%

THR	ASP	LEU	SER	SER	ALA	GLY	N483	A393	Y265	N184	S113	GLN
GLU	GLU	PRO	VAL	VAL	GLN	ARG	L488	D394	L272	L185	L114	CYS
MET	CYS	PRO	SER	SER	LEU	ILE	I397	V398	L273	R186	L115	VAL
ALA	SER	LYS	SER	ASN	THR	ALA	R494	I398	I281	F188	V117	ASN
GLN	LEU	PRO	ILE	LEU	PRO	THR	Y497	R399	I285	V189	N118	ILE
TYR	SER	SER	ILE	LEU	TRP	THR		E402	Y285	F190	N119	THR
LEU	LEU	VAL	ILE	LEU	ALA	ASP	G500	Q405	D290	I199	N122	ARG
GLN	GLN	ARG	TYR	VAL	VAL	ALA	H501	Q405		Y200	N123	T22
PRO	SER	THR	THR	THR	THR	VAL	V507	T411	T303	S201	V122	T26
LEU	GLY	PRO	MET	SER	SER	ARG		T411	VAL		C128	N27
LEU	SER	ILE	SER	THR	THR	ASP	G412	G412		I206	E129	S28
GLU	PHE	GLU	LEU	GLY	GLY	PRO	S510	T413	GLU	N207	F130	
GLY	CYS	GLY	GLY	SER	GLN	GLN	F511	T414	GLY	L208		R31
THR	THR	LEU	THR	ALA	ASN	THR	A415	A415	GLY	E209	P136	
ILE	GLN	VAL	GLU	VAL	VAL	LEU	A516	D416	ILE	R210	Y35	Y35
THR	LEU	PHE	ASN	PHE	GLN	GLU	P517	Y417	TYR	D211	D139	
SER	LEU	GLN	SER	SER	ILE	ILE		Y417	GLN	L212	V140	S57
GLY	ARG	VAL	VAL	VAL	THR	LEU	C521	K420	THR	L212		
TRP	VAL	ALA	ALA	ALA	ARG	ASP	G522	L421	SER	P213	TYR	W61
PHE	LEU	THR	SER	GLY	GLY	THR	P523	P422	ASN	F216	GLN	F62
GLY	GLY	ALA	ASN	CYS	THR	PRO	K524	D423	PHE	ASN	ASN	H63
ALA	ASP	LEU	GLY	THR	ILE	PRO	K525	D424	ARG	E220	ALA	H63
GLY	ALA	GLY	ILE	GLY	GLY	CYS	SER	G427	VAL	P221	LYS	ALA
PRO	GLY	PHE	ILE	GLY	GLY	PHE	ASN	G427	GLN	L222	LYS	ILE
LEU	LEU	ILE	ILE	GLY	ALA	GLY	LEU	K440	PRG	V223	TRP	VAL
GLN	LYS	ASP	PRO	VAL	TYR	VAL	LYS	Y445	GLU	I227	E150	GLY
ILE	GLN	THR	THR	THR	VAL	SER	ASN	M446	S321	G228	S151	THR
PRO	ASN	ASN	ASN	VAL	VAL	SER	LYS	Y447	R324	I229	S151	ASN
PHE	GLY	GLY	PHE	ASN	ILE	ILE	CYS	Y447		N230	R154	GLY
PRO	ASP	THR	THR	SER	THR	THR	VAL	R450	N330	T232	V156	LYS
MET	CYS	GLY	ILE	TYR	TYR	PRO	VAL	L451			S157	ARG
GLN	VAL	LEU	SER	GLY	GLY	GLY	ASN	F452	P333	Q235	S158	PHE
MET	PHE	GLY	VAL	THR	CYS	THR	PHE	R453		T236	A159	ASN
ALA	ALA	THR	THR	ASN	ASN	ASN	PHE	K454	N339	L237	N160	ASN
THR	ILE	GLN	THR	ILE	THR	THR	ASN	S455		L238	N161	PRO
ARG	ALA	VAL	GLU	PRO	ASN	GLY	GLY	V346	V346	A239	C162	ALA
PHE	ALA	LYS	ILE	VAL	ASN	SER	LEU	K456	LEU	L240	T163	LEU
ASN	ARG	GLN	LEU	GLN	GLY	GLN	THR	L457	N350	HIS	F164	PRO
GLY	ASP	PRO	PRO	VAL	ALA	VAL	GLY	D463	R351	ARG	E165	F83
ILE	LEU	VAL	VAL	GLY	ALA	VAL	THR	T464		SER	Y166	
GLY	ILE	GLY	SER	GLY	ILE	VAL	GLY	S465	I354	TYR	V167	Y88
VAL	CYS	THR	THR	THR	THR	LEU	VAL	T466	S355	LEU	S168	
THR	PRO	ALA	THR	THR	ALA	TYR	LEU	E467	V358	THR	Q169	
GLN	GLN	GLN	LYS	SER	GLN	GLN	THR	T468		PRO	P170	
ASN	LYS	ILE	ILE	ILE	GLY	GLY	GLU	Y469		GLY		
VAL	PHE	THR	VAL	VAL	VAL	VAL	SER	Q470	F367	ASP	M173	N96
LEU	ASN	THR	VAL	ASN	ASN	ASN	ASN	A471		SER		I97
TYR	PHE	GLY	ASP	GLN	CYS	CYS	LYS	F373		LEU		R99
GLY	LEU	LEU	CYS	GLY	THR	THR	LYS	K474		SER	GLU	G100
ASN	THR	THR	THR	LYS	GLY	GLY	PHE	P475	D385	GLY	W101	
GLN	VAL	VAL	MET	VAL	VAL	VAL	LEU	N476		THR	LYS	I102
LYS	ASN	THR	THR	THR	PRO	PRO	PRO	C477	L386	T255	GLY	F103
LEU	PHE	ILE	ILE	ALA	ALA	VAL	PHE	G478	C387	GLY	GLY	G104
ILE	PRO	PRO	CYS	GLY	VAL	VAL	GLN	V479	N390	A260	ASN	T105
ALA	LEU	LEU	GLY	GLY	ALA	ILE	GLN	P391	V392		PHE	
ASN	THR	THR	ASP	THR	ASP	THR	THR	D482		C764	V192	G112

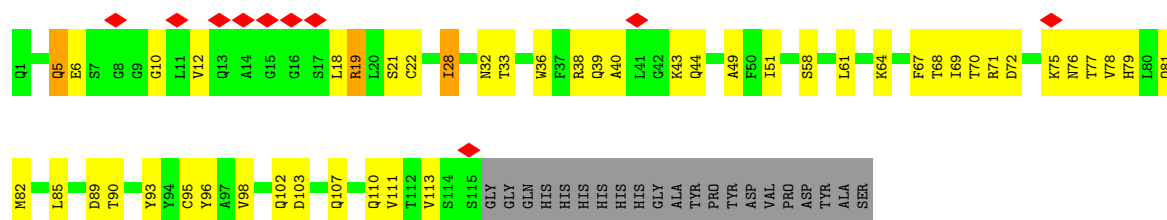
[illegible]

- Molecule 1: Spike glycoprotein

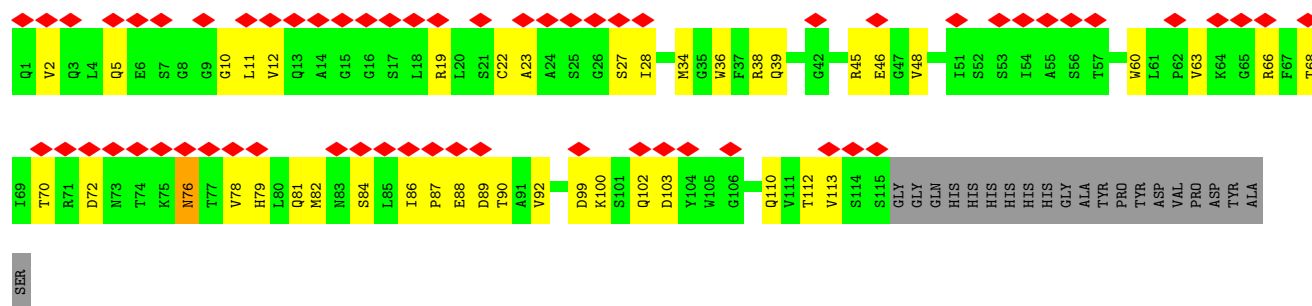


[illegible]

- Molecule 2: Nanosota-3C



- Molecule 2: Nanosota-3C



- Molecule 2: Nanosota-3C



I85	I86	P87	T90	A91	V92	Y93	Y94	D99	K100	G108	T112	V113	S114	S115	GLY	GLY	GLN	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLY	ALA	TYR	PRO	TYR	ASP	VAL	PRO	ASP	TYR	ALA	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	225916	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)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.655	Depositor
Minimum map value	-0.362	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0311	Depositor
Map size (Å)	339.96786, 339.96786, 339.96786	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.885333, 0.885333, 0.885333	Depositor



## 5 Model quality [i](#)

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

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	0.34	0/3611	0.53	1/4911 (0.0%)
1	B	0.34	0/3595	0.53	0/4888
1	C	0.32	0/3448	0.51	0/4688
2	D	0.30	0/897	0.57	0/1216
2	E	0.28	0/897	0.59	0/1216
2	L	0.35	0/897	0.68	0/1216
All	All	0.33	0/13345	0.54	1/18135 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ASP	CB-CG-OD1	5.87	123.58	118.30

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	3513	0	3396	102	0
1	B	3498	0	3378	105	0
1	C	3356	0	3251	76	0
2	D	879	0	855	46	0
2	E	879	0	855	28	0
2	L	879	0	855	40	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13004	0	12590	381	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 15.

The worst 5 of 381 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)
2:L:99:ASP:OD1	2:L:100:LYS:N	2.04	0.89
1:A:94:LYS:HE2	1:A:186:ARG:HH22	1.39	0.82
1:B:136:PRO:HD2	1:B:235:GLN:HE22	1.45	0.81
2:L:66:ARG:NH2	2:L:84:SER:O	2.13	0.81
2:E:2:VAL:HG12	2:E:27:SER:H	1.46	0.81

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	426/1230 (35%)	400 (94%)	26 (6%)	0	100	100
1	B	424/1230 (34%)	389 (92%)	33 (8%)	2 (0%)	25	59
1	C	403/1230 (33%)	386 (96%)	17 (4%)	0	100	100
2	D	113/136 (83%)	107 (95%)	5 (4%)	1 (1%)	14	49
2	E	113/136 (83%)	101 (89%)	11 (10%)	1 (1%)	14	49
2	L	113/136 (83%)	105 (93%)	7 (6%)	1 (1%)	14	49
All	All	1592/4098 (39%)	1488 (94%)	99 (6%)	5 (0%)	38	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	446	ASN
1	B	482	PRO
2	D	28	ILE
2	L	28	ILE
2	E	28	ILE

### 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	390/1070 (36%)	381 (98%)	9 (2%)	45	69
1	B	388/1070 (36%)	379 (98%)	9 (2%)	45	69
1	C	374/1070 (35%)	367 (98%)	7 (2%)	52	73
2	D	95/111 (86%)	92 (97%)	3 (3%)	34	62
2	E	95/111 (86%)	93 (98%)	2 (2%)	48	71
2	L	95/111 (86%)	93 (98%)	2 (2%)	48	71
All	All	1437/3543 (41%)	1405 (98%)	32 (2%)	47	70

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	76	ASN
2	E	82	MET
1	B	216	PHE
1	B	213	PRO
2	L	25	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	235	GLN
2	D	32	ASN
2	D	81	GLN
1	B	169	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	96	ASN

### 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](#)

There are no oligosaccharides in this entry.

### 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.

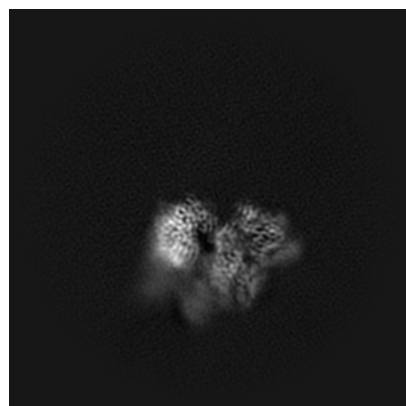
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43832. These allow visual inspection of the internal detail of the map and identification of artifacts.

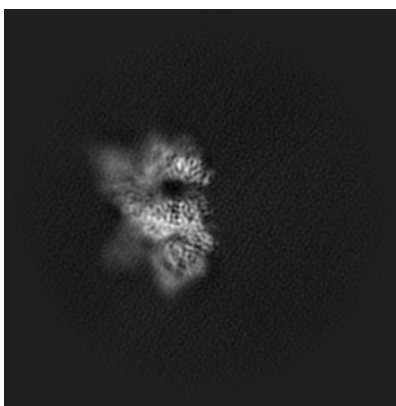
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

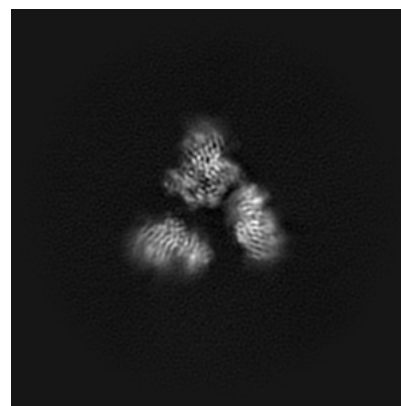
#### 6.1.1 Primary map



X

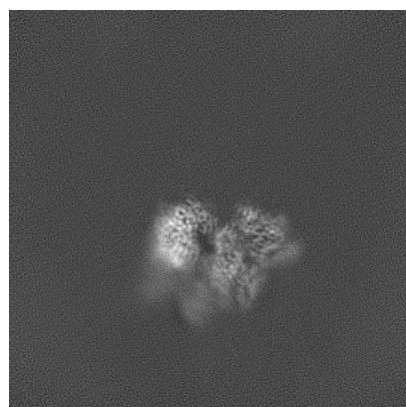


Y

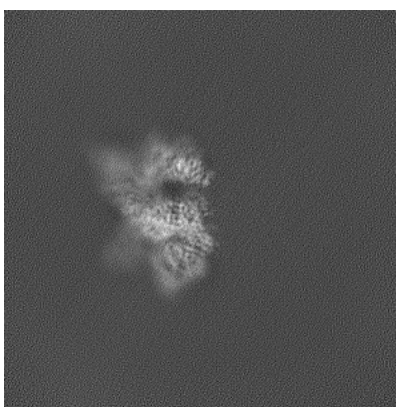


Z

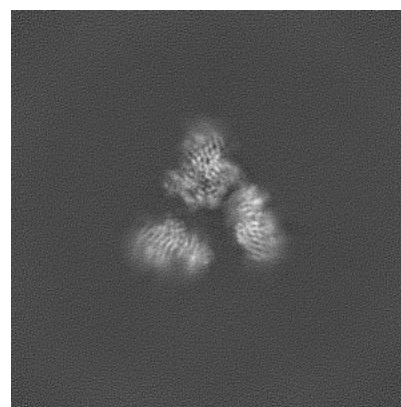
#### 6.1.2 Raw map



X



Y

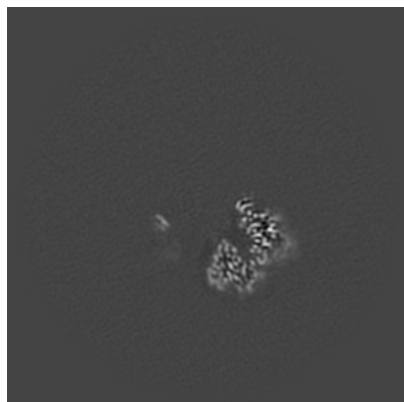


Z

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

## 6.2 Central slices [i](#)

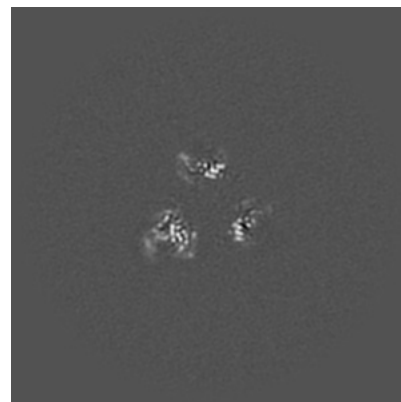
### 6.2.1 Primary map



X Index: 192

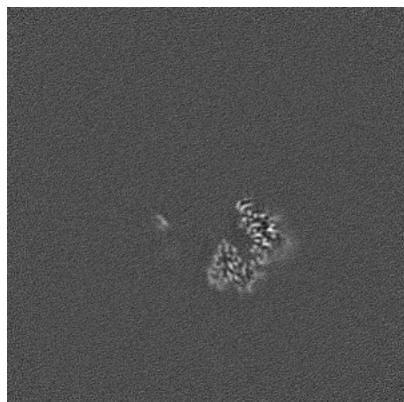


Y Index: 192



Z Index: 192

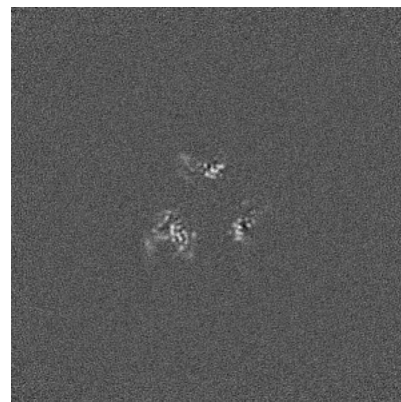
### 6.2.2 Raw map



X Index: 192



Y Index: 192



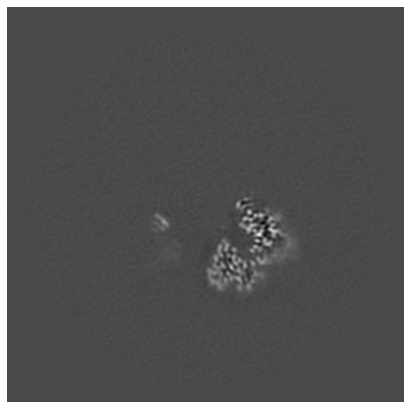
Z Index: 192

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

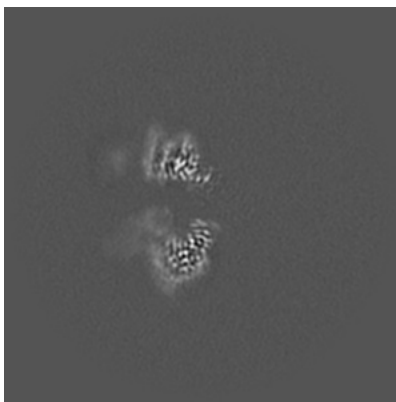


## 6.3 Largest variance slices [i](#)

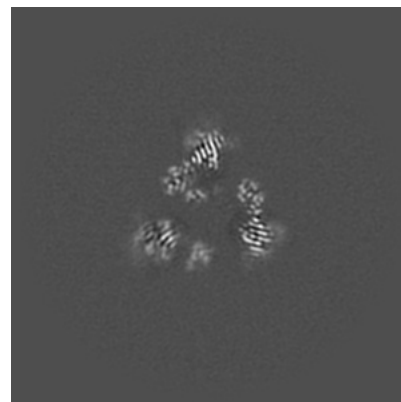
### 6.3.1 Primary map



X Index: 191

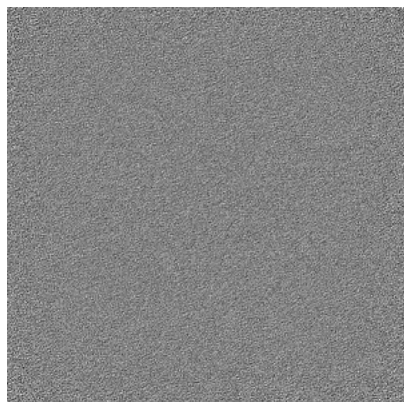


Y Index: 163

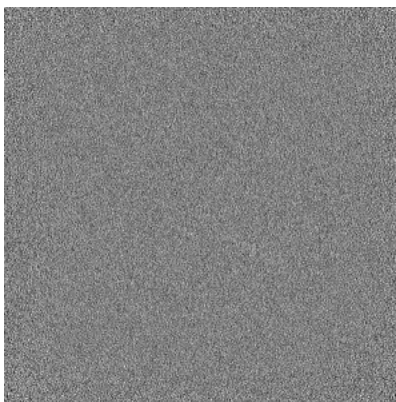


Z Index: 169

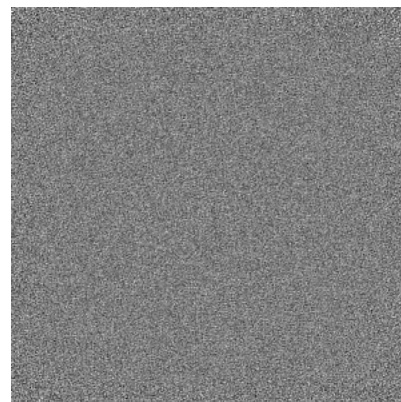
### 6.3.2 Raw map



X Index: 0



Y Index: 0



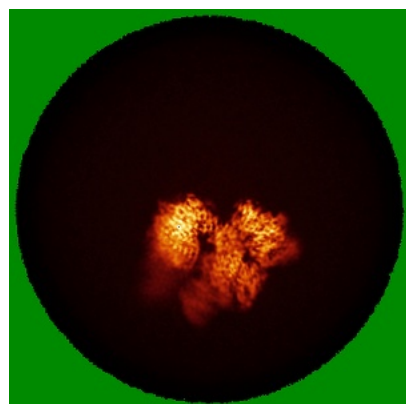
Z Index: 383

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

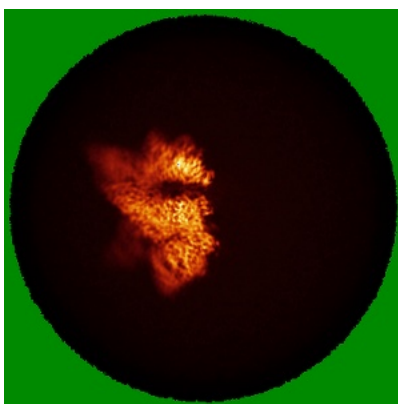


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

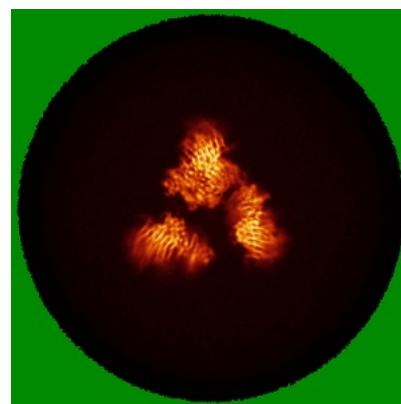
### 6.4.1 Primary map



X

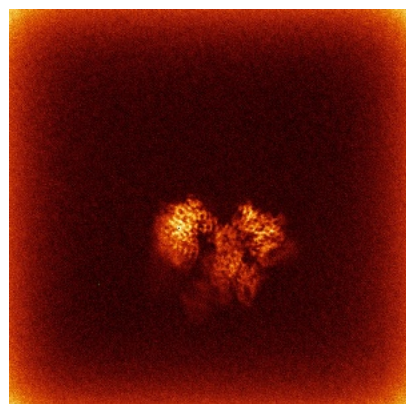


Y

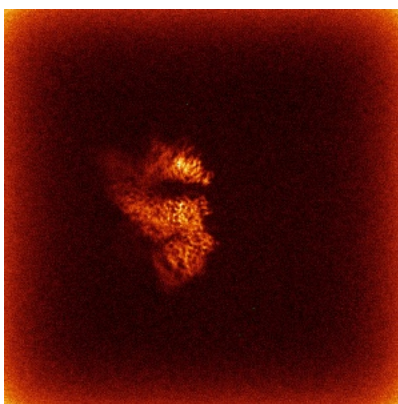


Z

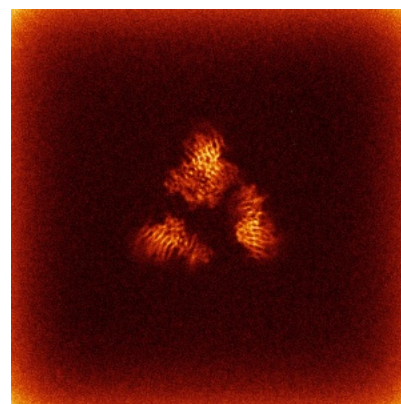
### 6.4.2 Raw map



X



Y

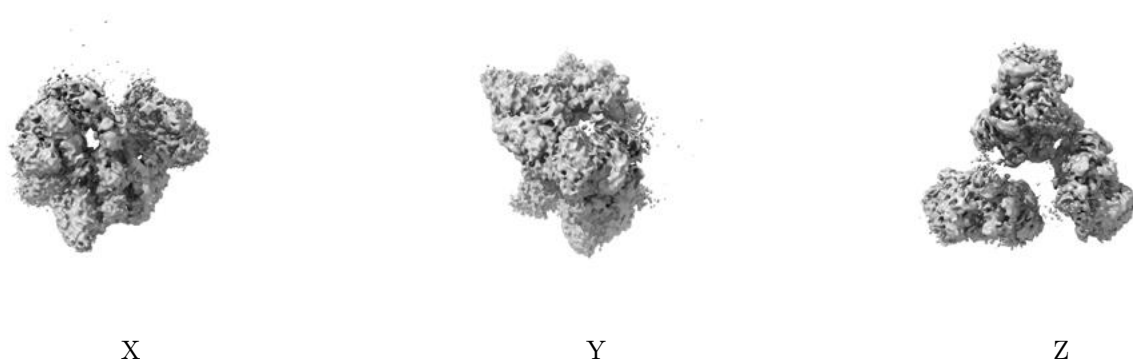


Z

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.

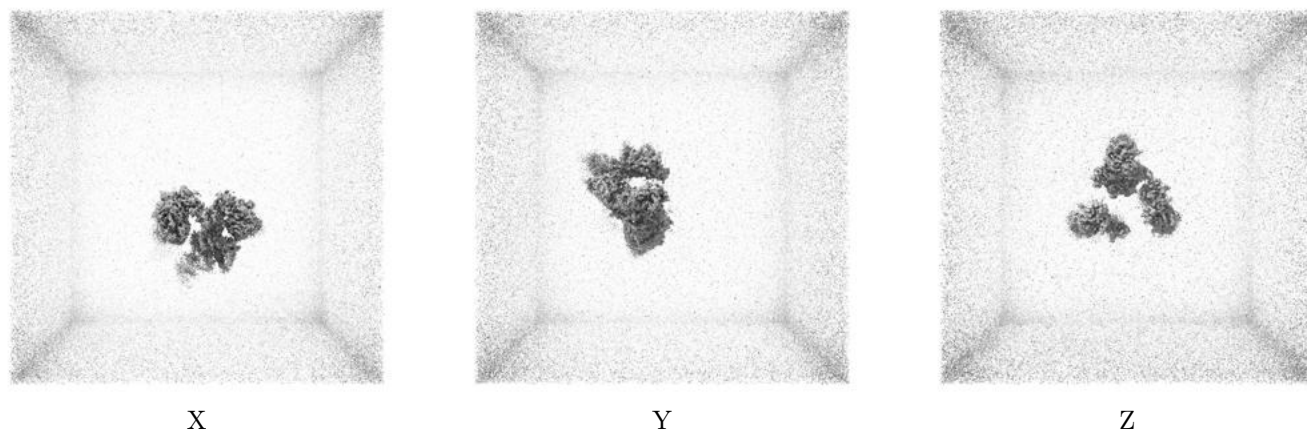
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0311. 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.

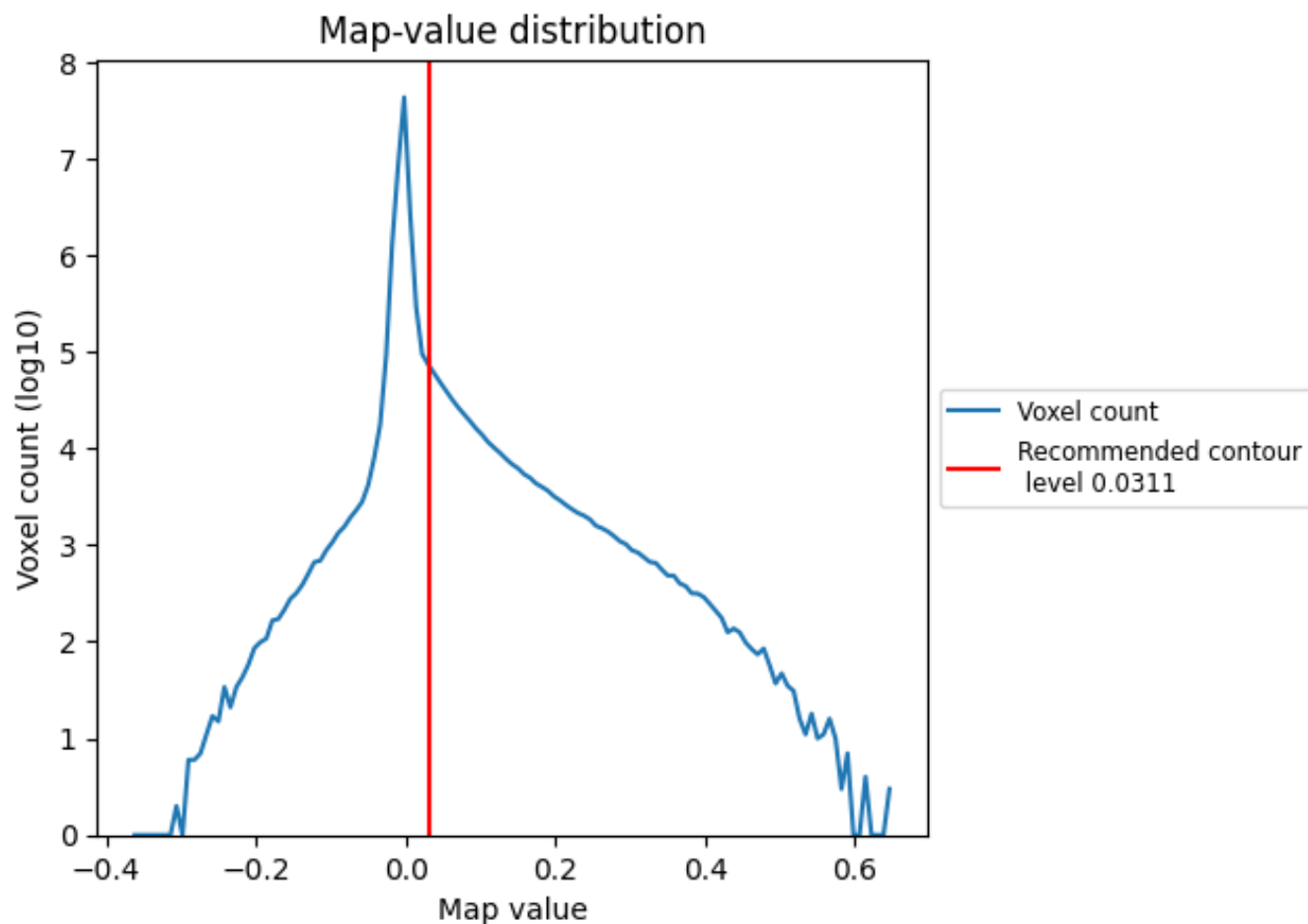
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

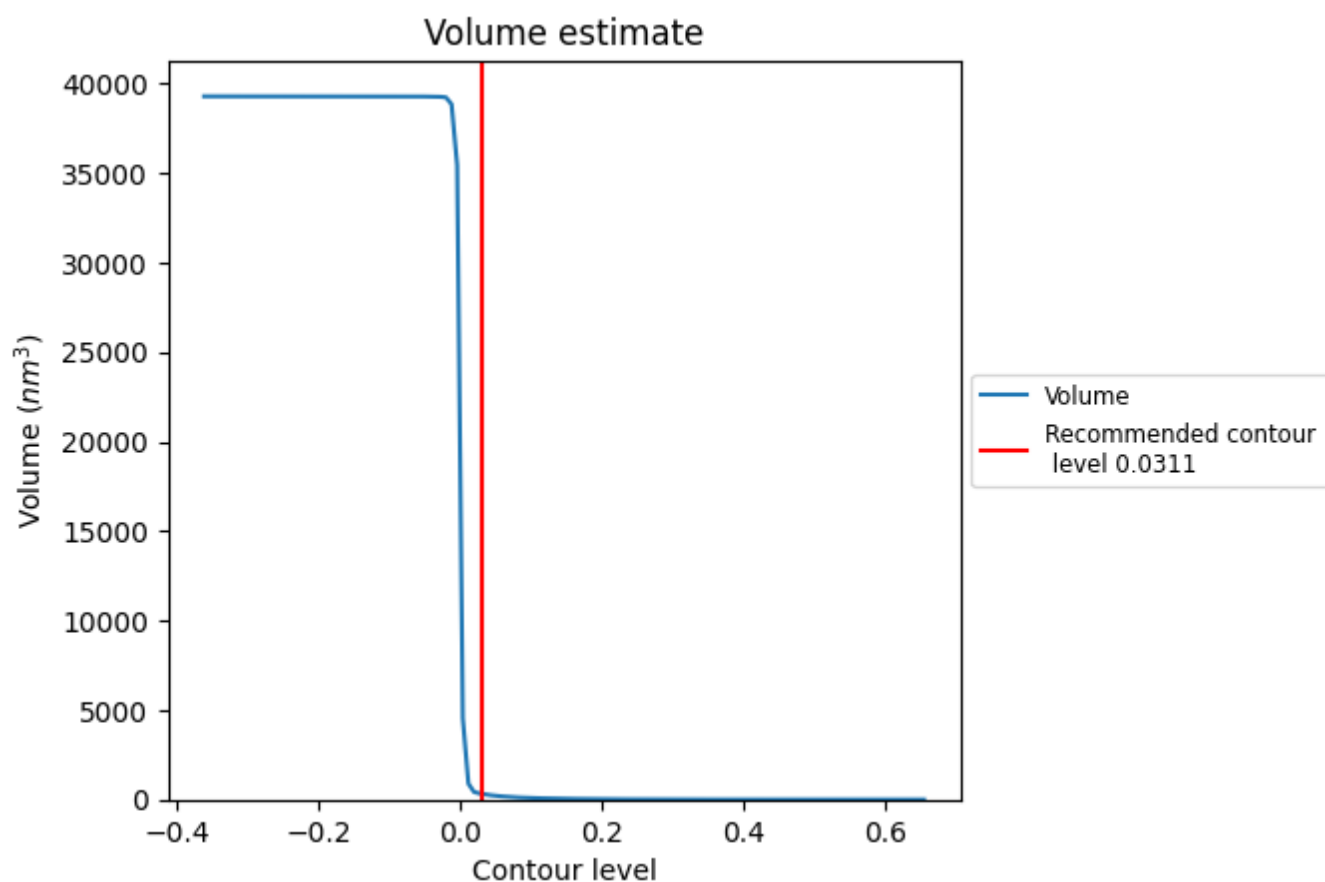
This section contains the results of statistical analysis of the map.

### 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.

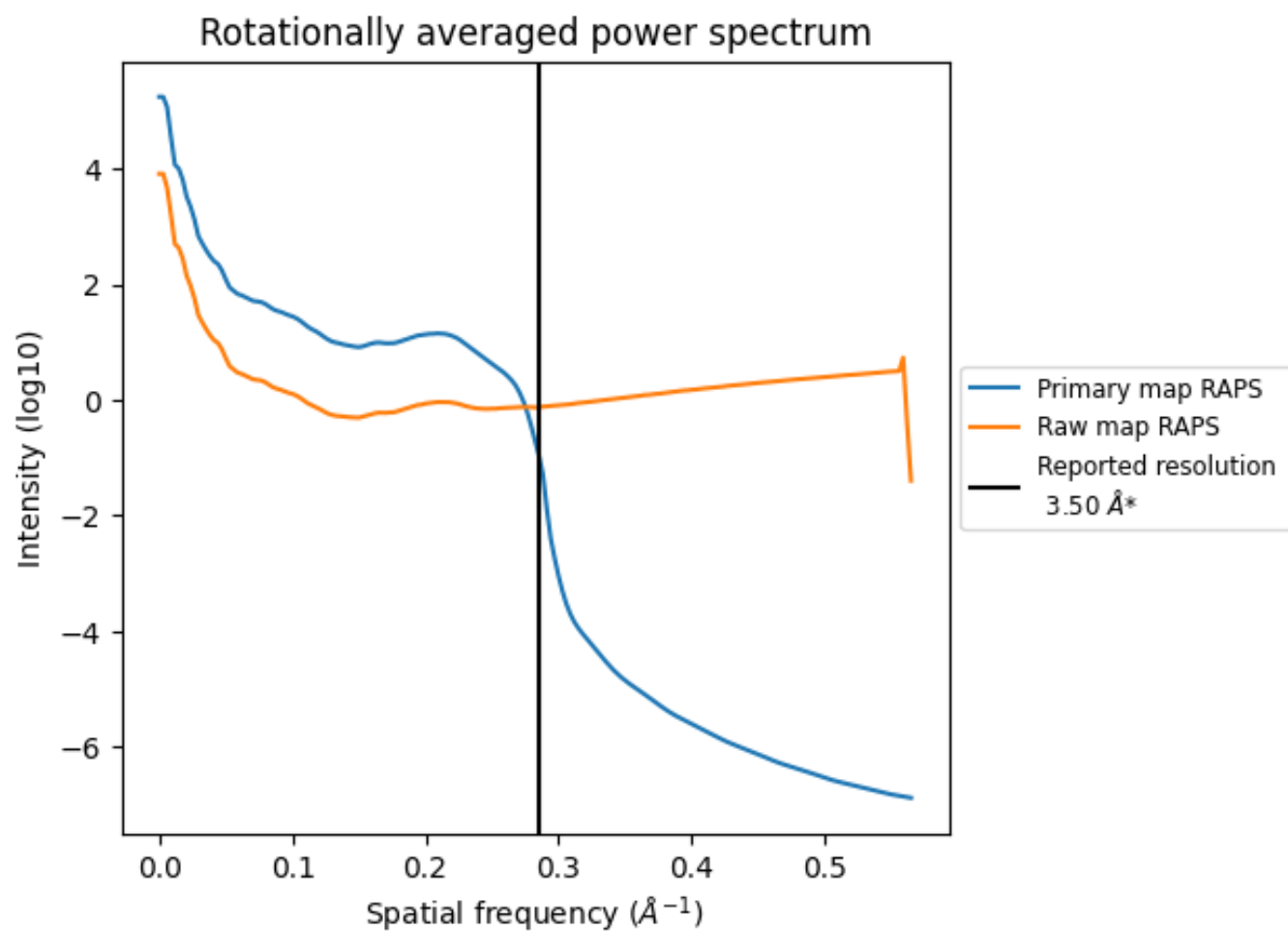
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 316  $\text{nm}^3$ ; this corresponds to an approximate mass of 285 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 ⓘ

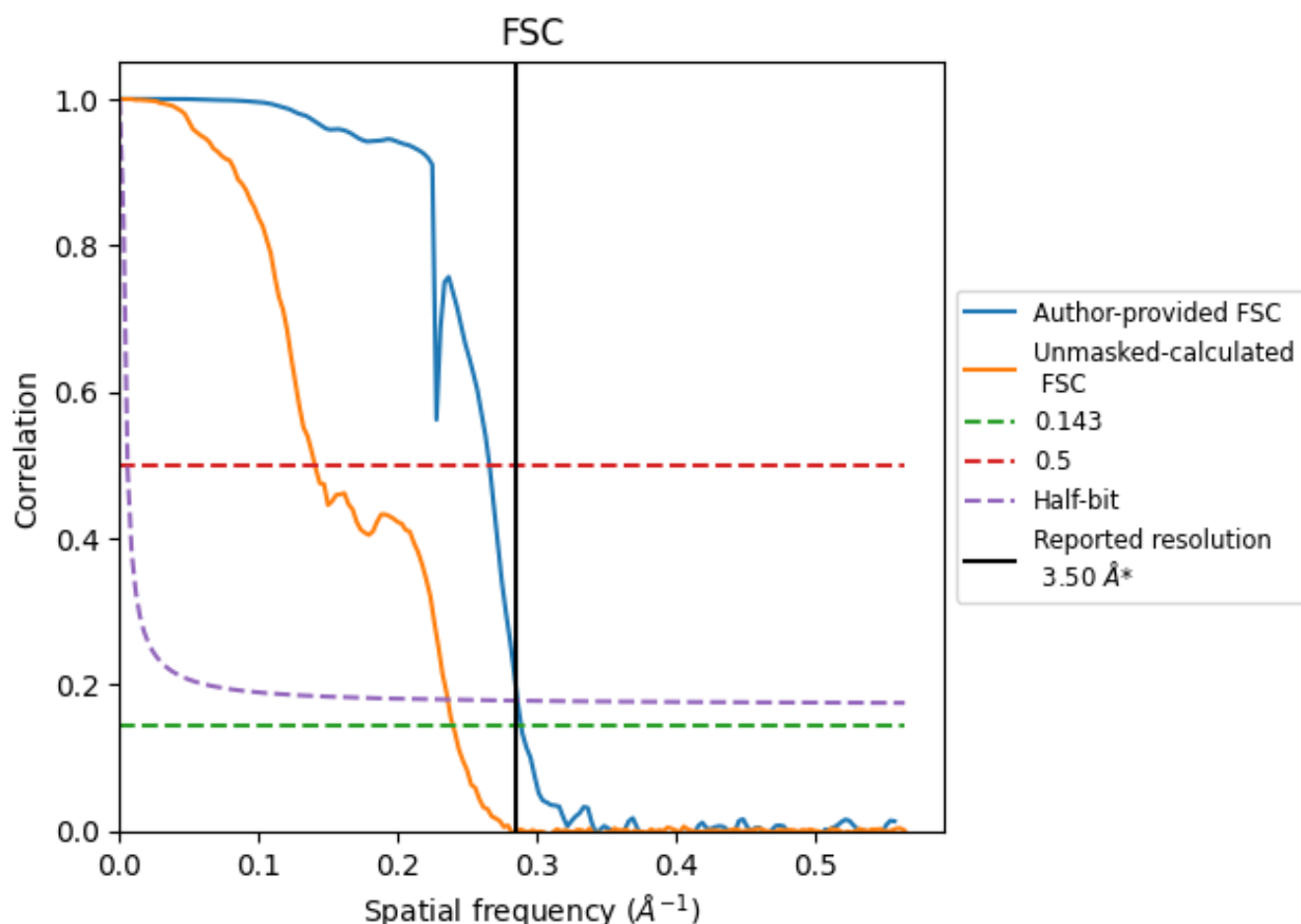


\*Reported resolution corresponds to spatial frequency of 0.286  $\text{\AA}^{-1}$

## 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 0.286  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.46	3.76	3.49
Unmasked-calculated*	4.17	7.12	4.24

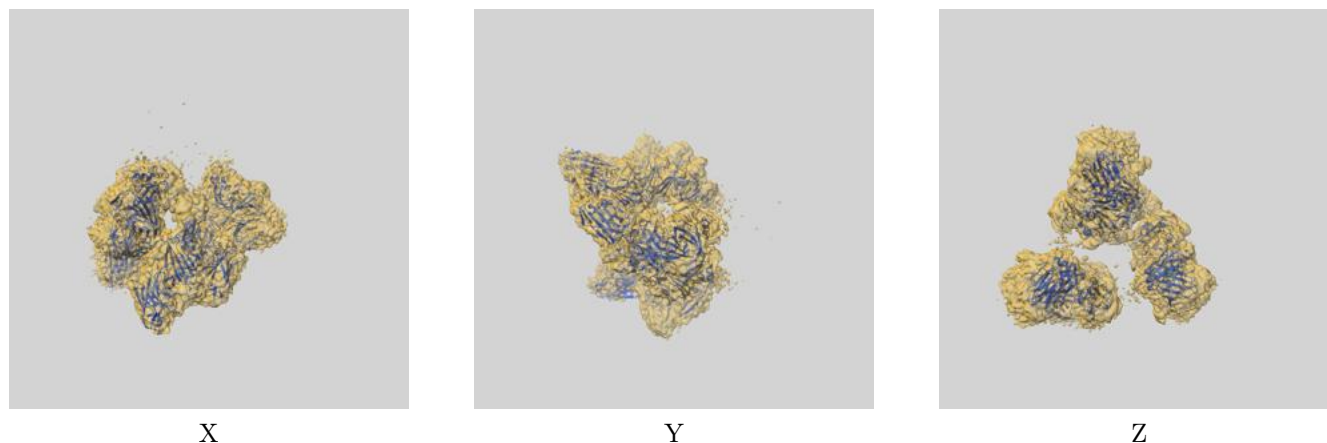
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.17 differs from the reported value 3.5 by more than 10 %



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

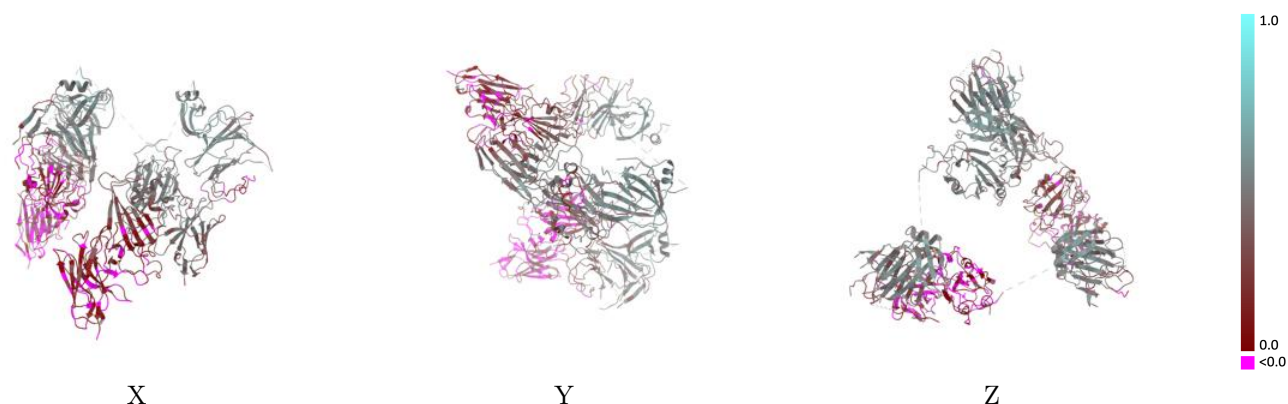
This section contains information regarding the fit between EMDB map EMD-43832 and PDB model 9ATP. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



The images above show the 3D surface view of the map at the recommended contour level 0.0311 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](#)



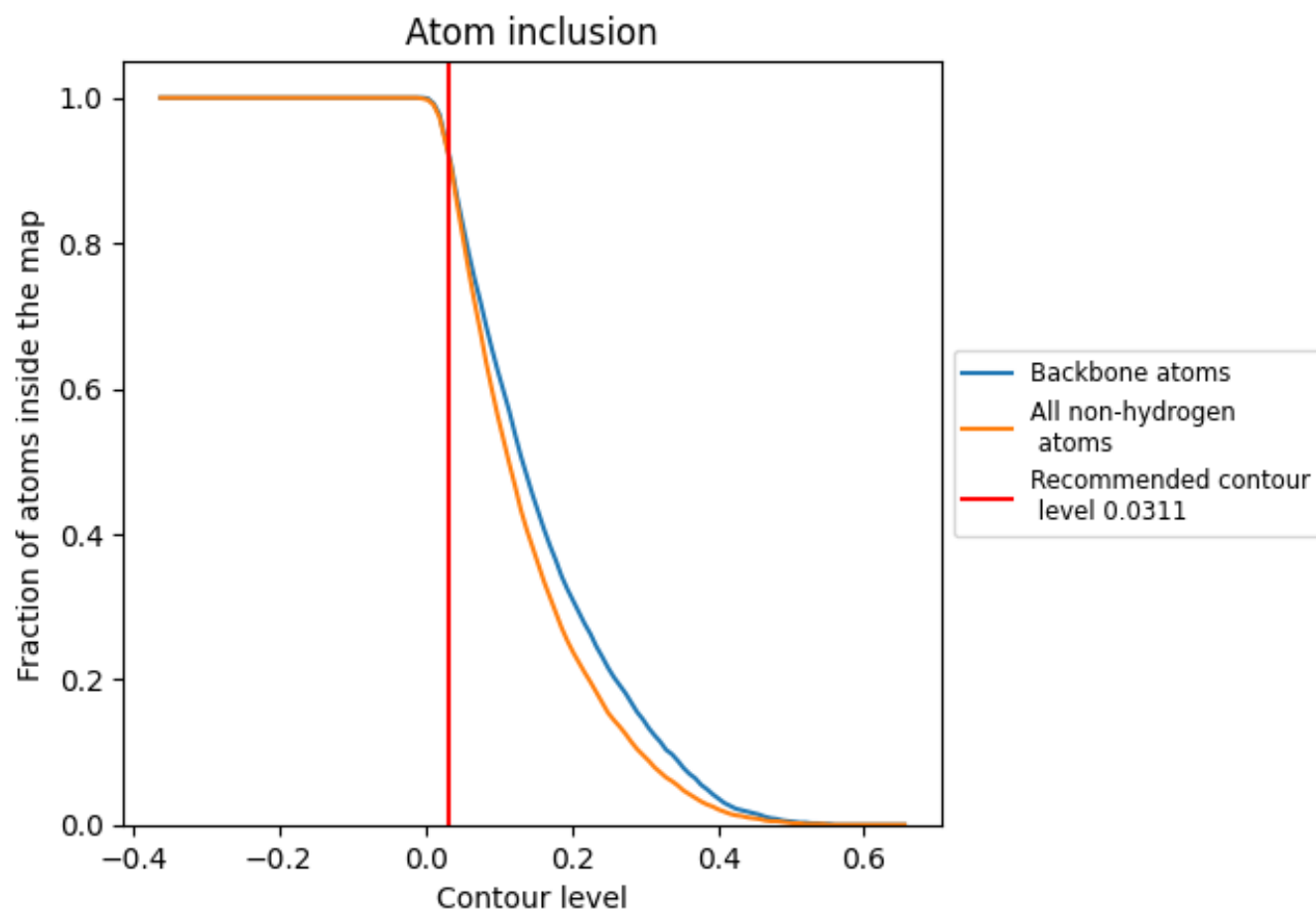
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0311).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.0311) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9240	<div><div></div></div> 0.3160
A	<div><div></div></div> 0.9630	<div><div></div></div> 0.3390
B	<div><div></div></div> 0.9920	<div><div></div></div> 0.4400
C	<div><div></div></div> 0.9240	<div><div></div></div> 0.2590
D	<div><div></div></div> 0.9070	<div><div></div></div> 0.1030
E	<div><div></div></div> 0.4470	<div><div></div></div> 0.0520
L	<div><div></div></div> 0.9950	<div><div></div></div> 0.4220

1.0

0.0

<0.0