



wwPDB EM Validation Summary Report ⓘ

Mar 4, 2026 – 10:10 PM UTC

PDB ID : 9CO9 / pdb_00009co9
EMDB ID : EMD-45774
Title : Local refinement of JN.1 spike/Nanosota-9 complex
Authors : Ye, G.; Bu, F.; Liu, B.; Li, F.
Deposited on : 2024-07-16
Resolution : 3.44 Å(reported)
Based on initial model : 8IOS

This is a wwPDB EM Validation Summary 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

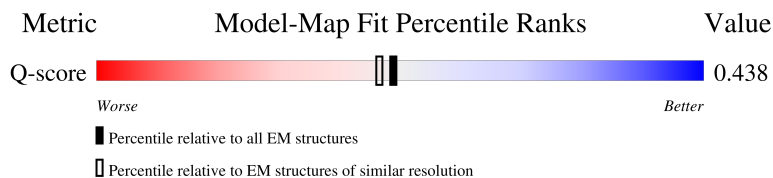
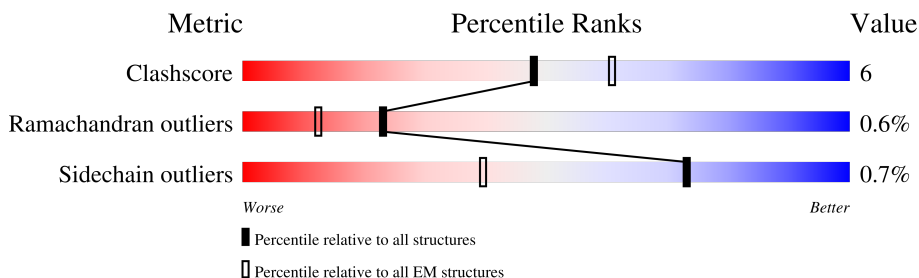
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.44 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13877 (2.94 - 3.94)

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	1243	 13% 84%
1	B	1243	 15% 84%
2	D	150	 44% 69% 15% 14%
2	E	150	 77% 9% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5198 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	B	200	Total	C	N	O	S	0	0
			1608	1042	270	288	8		
1	A	203	Total	C	N	O	S	0	0
			1634	1059	276	291	8		

There are 214 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	-	insertion	UNP P0DTC2
B	18	PRO	ASN	conflict	UNP P0DTC2
B	20	PHE	THR	conflict	UNP P0DTC2
B	21	ASN	THR	conflict	UNP P0DTC2
B	22	LEU	ARG	conflict	UNP P0DTC2
B	23	ILE	THR	conflict	UNP P0DTC2
B	24	THR	GLN	conflict	UNP P0DTC2
B	25	THR	LEU	conflict	UNP P0DTC2
B	26	THR	PRO	conflict	UNP P0DTC2
B	27	GLN	PRO	conflict	UNP P0DTC2
B	28	SER	ALA	conflict	UNP P0DTC2
B	51	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	126	PHE	VAL	conflict	UNP P0DTC2
B	141	ASP	GLY	conflict	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	155	SER	PHE	conflict	UNP P0DTC2
B	156	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	209	ILE	LEU	conflict	UNP P0DTC2
B	210	GLY	VAL	conflict	UNP P0DTC2
B	213	PHE	LEU	conflict	UNP P0DTC2
B	242	ASN	HIS	conflict	UNP P0DTC2
B	261	ASP	ALA	conflict	UNP P0DTC2
B	329	VAL	ILE	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	336	HIS	GLY	conflict	UNP P0DTC2
B	353	THR	LYS	conflict	UNP P0DTC2
B	368	PHE	SER	conflict	UNP P0DTC2
B	370	PRO	SER	conflict	UNP P0DTC2
B	372	PHE	SER	conflict	UNP P0DTC2
B	373	ALA	THR	conflict	UNP P0DTC2
B	400	LYS	ARG	conflict	UNP P0DTC2
B	402	ASN	ASP	conflict	UNP P0DTC2
B	405	SER	ARG	conflict	UNP P0DTC2
B	414	ASN	LYS	conflict	UNP P0DTC2
B	437	LYS	ASN	conflict	UNP P0DTC2
B	442	HIS	VAL	conflict	UNP P0DTC2
B	443	SER	GLY	conflict	UNP P0DTC2
B	447	ASP	ASN	conflict	UNP P0DTC2
B	449	TRP	LEU	conflict	UNP P0DTC2
B	452	SER	LEU	conflict	UNP P0DTC2
B	457	LYS	ASN	conflict	UNP P0DTC2
B	474	ASN	SER	conflict	UNP P0DTC2
B	475	LYS	THR	conflict	UNP P0DTC2
B	478	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	480	LYS	GLU	conflict	UNP P0DTC2
B	482	PRO	PHE	conflict	UNP P0DTC2
B	494	ARG	GLN	conflict	UNP P0DTC2
B	497	TYR	ASN	conflict	UNP P0DTC2
B	501	HIS	TYR	conflict	UNP P0DTC2
B	550	LYS	GLU	conflict	UNP P0DTC2
B	566	VAL	ALA	conflict	UNP P0DTC2
B	610	GLY	ASP	conflict	UNP P0DTC2
B	617	SER	PRO	conflict	UNP P0DTC2
B	651	TYR	HIS	conflict	UNP P0DTC2
B	675	LYS	ASN	conflict	UNP P0DTC2
B	677	ARG	PRO	conflict	UNP P0DTC2
B	678	ALA	ARG	conflict	UNP P0DTC2
B	679	GLY	ARG	conflict	UNP P0DTC2
B	760	LYS	ASN	conflict	UNP P0DTC2
B	792	TYR	ASP	conflict	UNP P0DTC2
B	813	PRO	PHE	conflict	UNP P0DTC2
B	888	PRO	ALA	conflict	UNP P0DTC2
B	895	PRO	ALA	conflict	UNP P0DTC2
B	935	PHE	SER	conflict	UNP P0DTC2
B	938	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	950	HIS	GLN	conflict	UNP P0DTC2
B	965	LYS	ASN	conflict	UNP P0DTC2
B	982	PRO	LYS	conflict	UNP P0DTC2
B	983	PRO	VAL	conflict	UNP P0DTC2
B	1139	LEU	PRO	conflict	UNP P0DTC2
B	1208	GLY	TRP	conflict	UNP P0DTC2
B	1209	SER	PRO	conflict	UNP P0DTC2
B	1210	GLY	TRP	conflict	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
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
A	17	MET	-	insertion	UNP P0DTC2
A	18	PRO	ASN	conflict	UNP P0DTC2
A	20	PHE	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ASN	THR	conflict	UNP P0DTC2
A	22	LEU	ARG	conflict	UNP P0DTC2
A	23	ILE	THR	conflict	UNP P0DTC2
A	24	THR	GLN	conflict	UNP P0DTC2
A	25	THR	LEU	conflict	UNP P0DTC2
A	26	THR	PRO	conflict	UNP P0DTC2
A	27	GLN	PRO	conflict	UNP P0DTC2
A	28	SER	ALA	conflict	UNP P0DTC2
A	51	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	126	PHE	VAL	conflict	UNP P0DTC2
A	141	ASP	GLY	conflict	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	155	SER	PHE	conflict	UNP P0DTC2
A	156	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	209	ILE	LEU	conflict	UNP P0DTC2
A	210	GLY	VAL	conflict	UNP P0DTC2
A	213	PHE	LEU	conflict	UNP P0DTC2
A	242	ASN	HIS	conflict	UNP P0DTC2
A	261	ASP	ALA	conflict	UNP P0DTC2
A	329	VAL	ILE	conflict	UNP P0DTC2
A	336	HIS	GLY	conflict	UNP P0DTC2
A	353	THR	LYS	conflict	UNP P0DTC2
A	368	PHE	SER	conflict	UNP P0DTC2
A	370	PRO	SER	conflict	UNP P0DTC2
A	372	PHE	SER	conflict	UNP P0DTC2
A	373	ALA	THR	conflict	UNP P0DTC2
A	400	LYS	ARG	conflict	UNP P0DTC2
A	402	ASN	ASP	conflict	UNP P0DTC2
A	405	SER	ARG	conflict	UNP P0DTC2
A	414	ASN	LYS	conflict	UNP P0DTC2
A	437	LYS	ASN	conflict	UNP P0DTC2
A	442	HIS	VAL	conflict	UNP P0DTC2
A	443	SER	GLY	conflict	UNP P0DTC2
A	447	ASP	ASN	conflict	UNP P0DTC2
A	449	TRP	LEU	conflict	UNP P0DTC2
A	452	SER	LEU	conflict	UNP P0DTC2
A	457	LYS	ASN	conflict	UNP P0DTC2
A	474	ASN	SER	conflict	UNP P0DTC2
A	475	LYS	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	478	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	480	LYS	GLU	conflict	UNP P0DTC2
A	482	PRO	PHE	conflict	UNP P0DTC2
A	494	ARG	GLN	conflict	UNP P0DTC2
A	497	TYR	ASN	conflict	UNP P0DTC2
A	501	HIS	TYR	conflict	UNP P0DTC2
A	550	LYS	GLU	conflict	UNP P0DTC2
A	566	VAL	ALA	conflict	UNP P0DTC2
A	610	GLY	ASP	conflict	UNP P0DTC2
A	617	SER	PRO	conflict	UNP P0DTC2
A	651	TYR	HIS	conflict	UNP P0DTC2
A	675	LYS	ASN	conflict	UNP P0DTC2
A	677	ARG	PRO	conflict	UNP P0DTC2
A	678	ALA	ARG	conflict	UNP P0DTC2
A	679	GLY	ARG	conflict	UNP P0DTC2
A	760	LYS	ASN	conflict	UNP P0DTC2
A	792	TYR	ASP	conflict	UNP P0DTC2
A	813	PRO	PHE	conflict	UNP P0DTC2
A	888	PRO	ALA	conflict	UNP P0DTC2
A	895	PRO	ALA	conflict	UNP P0DTC2
A	935	PHE	SER	conflict	UNP P0DTC2
A	938	PRO	ALA	conflict	UNP P0DTC2
A	950	HIS	GLN	conflict	UNP P0DTC2
A	965	LYS	ASN	conflict	UNP P0DTC2
A	982	PRO	LYS	conflict	UNP P0DTC2
A	983	PRO	VAL	conflict	UNP P0DTC2
A	1139	LEU	PRO	conflict	UNP P0DTC2
A	1208	GLY	TRP	conflict	UNP P0DTC2
A	1209	SER	PRO	conflict	UNP P0DTC2
A	1210	GLY	TRP	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	ARG	-	expression tag	UNP P0DTC2
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

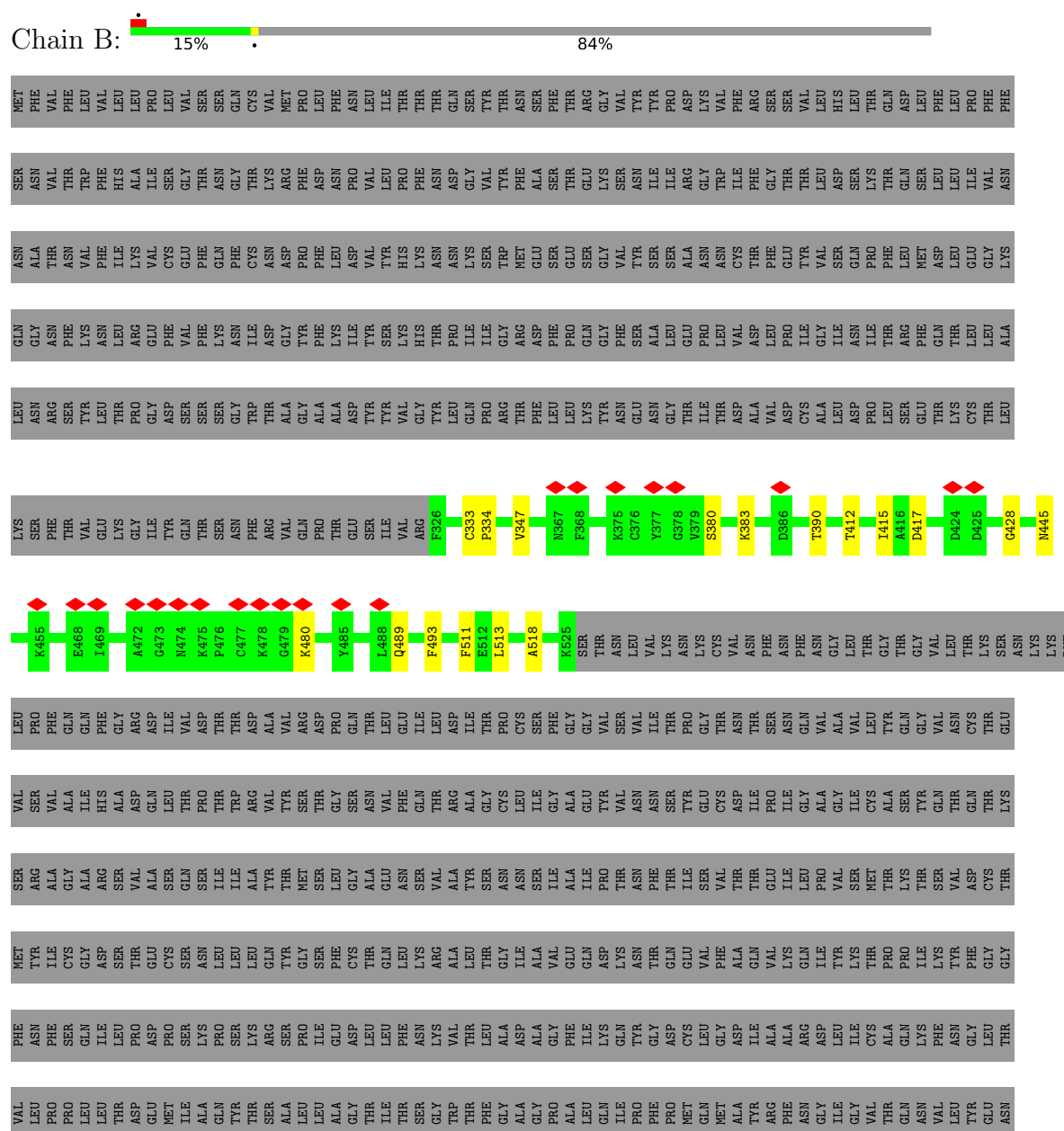
- Molecule 2 is a protein called Nanosota-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	129	Total	C	N	O	S	0	0
			978	602	168	203	5		
2	E	129	Total	C	N	O	S	0	0
			978	602	168	203	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]

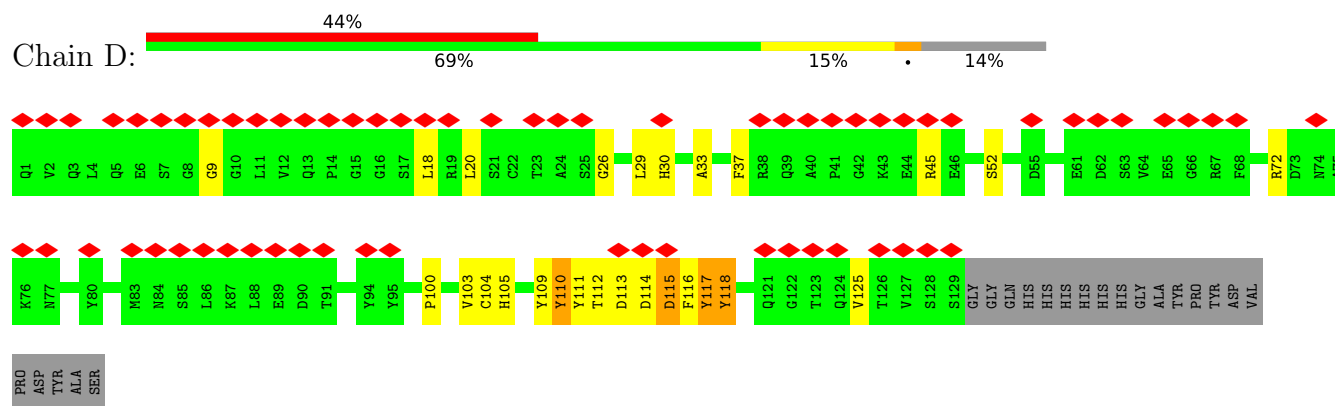
- Molecule 1: Spike glycoprotein

Chain A: 13% . 84%

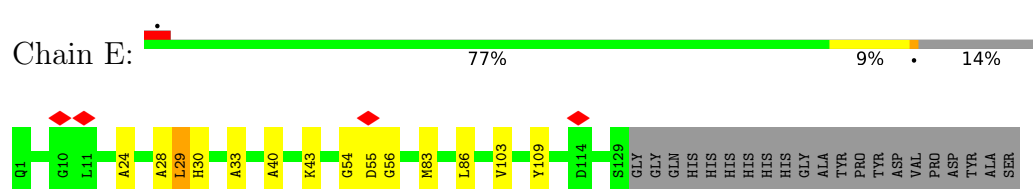
ILE	THR	THR	GLY	LYS	GLN	LYS	LEU	GLN	ASN	SER	MET
THR	SER	GLN	VAL	SER	ASN	SER	ASN	GLY	ALA	ASN	PHE
SER	VAL	THR	ASN	ASN	THR	PHE	THR	ASN	THR	VAL	THR
ASP	GLN	THR	CYS	LYS	THR	VAL	TYR	PHE	ASN	VAL	THR
THR	LYS	THR	GLY	PHE	LEU	GLU	LEU	ASN	PHE	ILE	VAL
MET	SER	VAL	VAL	LEU	VAL	LYS	THR	LEU	ILE	HIS	VAL
TYR	ARG	ARG	SER	PRO	SER	GLY	PRO	ARG	LYS	ALA	LEU
ILE	ALA	ALA	VAL	PHE	ILE	ILE	GLY	GLY	VAL	VAL	PRO
THR	CYS	GLY	ALA	GLN	GLN	TYR	SER	PHE	CYS	SER	LEU
GLY	ALA	ALA	ILE	PHE	GLN	GLN	SER	VAL	GLY	VAL	VAL
ASP	ARG	ARG	HIS	GLN	THR	THR	SER	SER	THR	THR	SER
SER	SER	SER	ALA	GLY	GLY	K478	GLN	SER	GLN	ASN	SER
THR	THR	VAL	ASP	ASP	ASP	G431	PHE	ASN	PHE	GLY	SER
GLU	GLU	ALA	GLN	ARG	THR	THR	ARG	THR	THR	TRP	THR
CYS	SER	SER	LEU	ILE	VAL	VAL	VAL	ARG	ALA	ALA	VAL
ASN	ASN	SER	PRO	ASP	THR	THR	GLN	GLN	PRO	GLY	PRO
LEU	LEU	ILE	THR	THR	THR	THR	THR	THR	PHE	PHE	LEU
LEU	LEU	ALA	ARG	ASP	ALA	ASP	GLU	ASP	LEU	ASN	PHE
ARG	GLN	TYR	VAL	VAL	VAL	R494	SER	ASN	VAL	VAL	LEU
SER	TYR	THR	SER	VAL	VAL	Y497	I223	TYR	TYR	VAL	ILE
PRO	GLY	MET	SER	ARG	ASP	Y497	I223	SER	TYR	VAL	ILE
ILE	SER	SER	THR	ASP	THR	R505	T330	GLY	HIS	PRO	THR
GLU	PHE	GLY	GLY	GLN	GLY	R505	T330	THR	LYS	PHE	THR
ASP	CYS	GLY	SER	PRO	SER	V508	C333	LEU	ASN	ASN	THR
LEU	LEU	ALA	THR	THR	ASN	P334	P334	GLN	ASN	GLN	SER
PHE	LEU	ASN	PHE	GLY	LEU	H515	F335	ARG	SER	VAL	TYR
ASN	SER	GLN	GLN	ILE	ILE	A516	F339	THR	MET	TYR	THR
LYS	ARG	VAL	THR	LEU	LEU	P517	N340	PHE	ALA	ALA	ASN
VAL	ALA	ALA	ARG	ASP	ASP	A516	F339	THR	SER	SER	PHE
THR	LEU	LEU	ALA	ASP	ALA	P517	N340	ASP	THR	THR	THR
LEU	THR	SER	GLY	ILE	ILE	V520	Y347	LEU	GLY	GLY	ARG
GLY	THR	ASN	CYS	PRO	PRO	C521	Y348	LEU	VAL	GLY	ARG
ALA	ILE	ASN	LEU	THR	LEU	C521	A349	ASN	GLY	VAL	GLY
ASP	ILE	ASN	LEU	CYS	THR	K625	F368	THR	ASN	GLY	LYS
ALA	SER	SER	ILE	SER	SER	SER	C358	GLU	SER	TRP	VAL
ALA	ALA	ALA	GLY	PHE	THR	THR	Y362	GLY	ALA	ILE	PHE
GLY	GLY	ALA	ALA	GLY	GLY	ASN	Y362	GLY	SER	ILE	THR
PHE	GLU	ILE	GLY	GLY	VAL	VAL	F368	THR	ALA	ARG	PRO
LYS	ASP	PRO	TYR	VAL	SER	LYS	F368	ILE	ASN	GLY	LYS
GLN	ASN	THR	VAL	SER	VAL	LYS	F368	THR	ASN	TRP	VAL
TYR	ASN	ASN	ASN	VAL	ASN	ASN	K383	ASP	CYS	ILE	PHE
GLY	THR	PHE	ASN	ILE	GLN	LYS	L384	ALA	THR	THR	VAL
ASP	THR	THR	SER	THR	THR	CYS	C388	VAL	GLY	THR	SER
CYS	ILE	ILE	TYR	PRO	VAL	VAL	C388	ASP	PRO	THR	VAL
LEU	VAL	SER	GLY	THR	ASN	ASN	F389	CYS	TYR	THR	THR
F389	VAL	THR	PHE	THR	PHE	PHE	T390	ALA	GLY	GLY	LEU
ASN	ASN	ASN	ASN	ASN	ASN	H391	R391	LEU	ASN	ASN	LEU
VAL	VAL	SER	PHE	SER	ASN	V392	V392	PRO	LYS	THR	THR
ALA	ASN	ASN	GLY	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN	ASN	ASN	ASN	ASN	V392	V392	ASN	THR	PHE	GLN
ALA	ASN										

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

- Molecule 2: Nanosota-9



- Molecule 2: Nanosota-9



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	248315	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.8	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.090	Depositor
Minimum map value	-0.374	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.12	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

5.1 Standard geometry

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	0.50	0/1688	0.74	1/2296 (0.0%)
1	B	0.19	0/1662	0.48	0/2261
2	D	0.36	0/998	0.73	2/1353 (0.1%)
2	E	0.27	0/998	0.53	0/1353
All	All	0.36	0/5346	0.63	3/7263 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	30	HIS	N-CA-C	-7.67	102.99	114.64
1	A	339	PHE	CA-CB-CG	6.28	120.08	113.80
2	D	110	TYR	CA-CB-CG	5.33	123.49	113.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	494	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1634	0	1564	25	0
1	B	1608	0	1531	11	0
2	D	978	0	905	18	0
2	E	978	0	905	8	0
All	All	5198	0	4905	60	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.

The worst 5 of 60 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:418:TYR:HD2	1:A:454:ARG:HB2	1.47	0.79
1:A:481:GLY:H	1:A:484:CYS:HB2	1.52	0.74
2:D:33:ALA:HB3	2:D:103:VAL:HG12	1.74	0.68
2:D:105:HIS:HB2	2:D:110:TYR:HD1	1.59	0.67
1:A:418:TYR:CD2	1:A:454:ARG:HB2	2.30	0.66

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	201/1243 (16%)	190 (94%)	10 (5%)	1 (0%)	24	56
1	B	198/1243 (16%)	188 (95%)	10 (5%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	127/150 (85%)	115 (91%)	10 (8%)	2 (2%)	7	33
2	E	127/150 (85%)	115 (91%)	11 (9%)	1 (1%)	16	47
All	All	653/2786 (23%)	608 (93%)	41 (6%)	4 (1%)	23	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	115	ASP
2	D	118	TYR
2	E	55	ASP
1	A	333	CYS

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	177/1085 (16%)	175 (99%)	2 (1%)	65	74
1	B	174/1085 (16%)	174 (100%)	0	100	100
2	D	104/120 (87%)	103 (99%)	1 (1%)	68	75
2	E	104/120 (87%)	103 (99%)	1 (1%)	68	75
All	All	559/2410 (23%)	555 (99%)	4 (1%)	73	78

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	454	ARG
1	A	465	ILE
2	D	117	TYR
2	E	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	406	GLN
1	B	414	ASN
1	B	442	HIS
1	B	489	GLN
1	A	385	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.

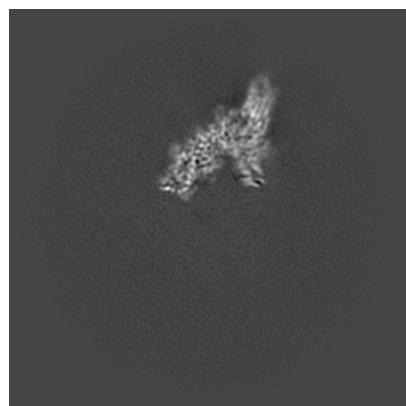
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45774. These allow visual inspection of the internal detail of the map and identification of artifacts.

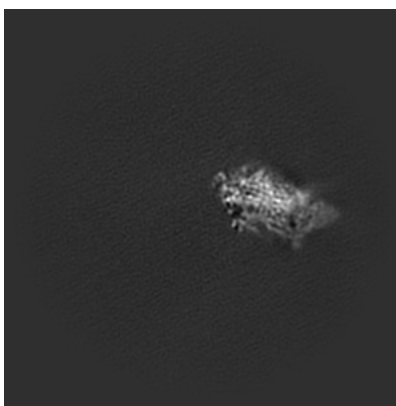
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

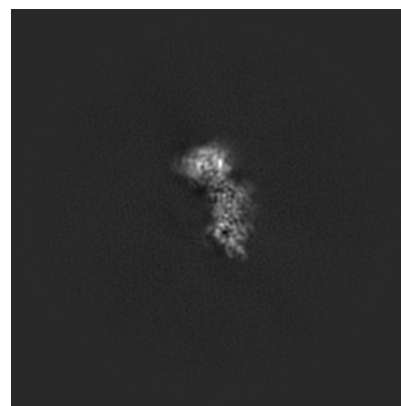
6.1.1 Primary map



X

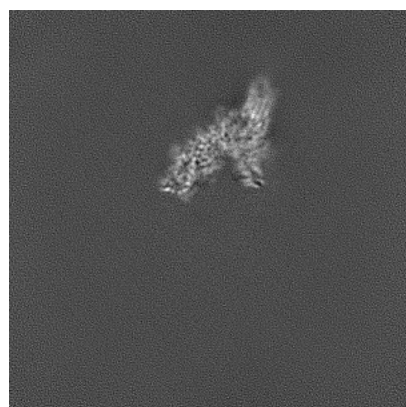


Y

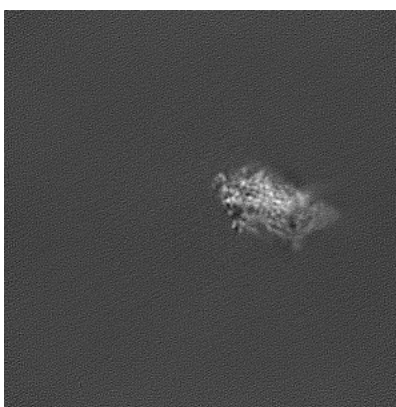


Z

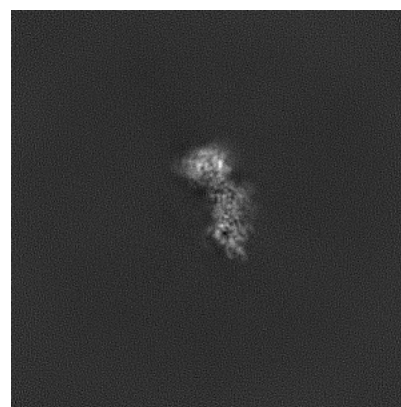
6.1.2 Raw map



X



Y

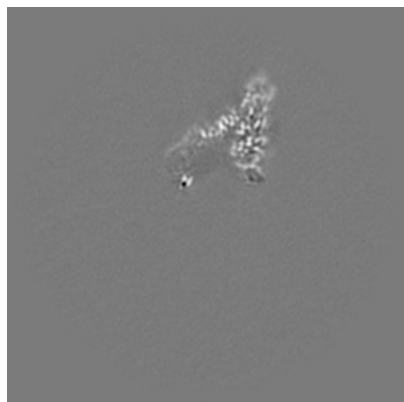


Z

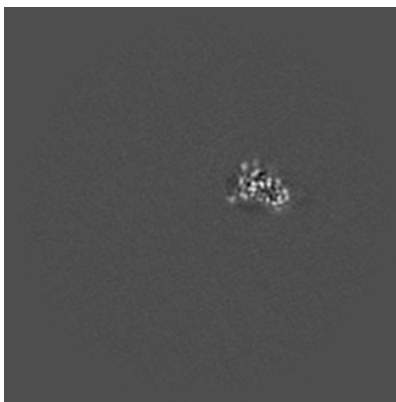
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

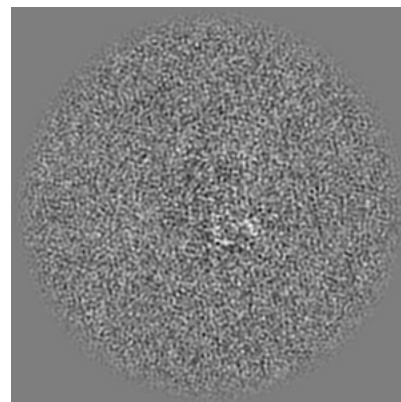
6.2.1 Primary map



X Index: 192

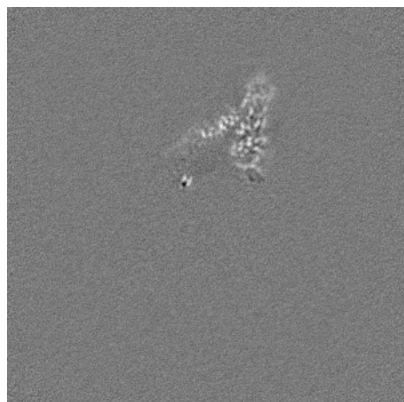


Y Index: 192

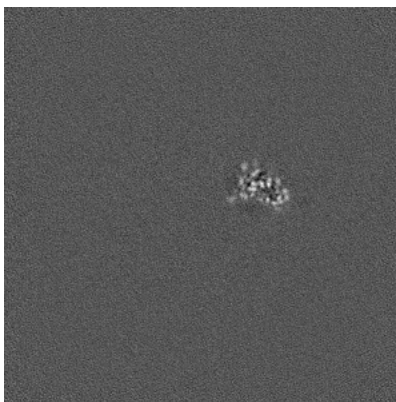


Z Index: 192

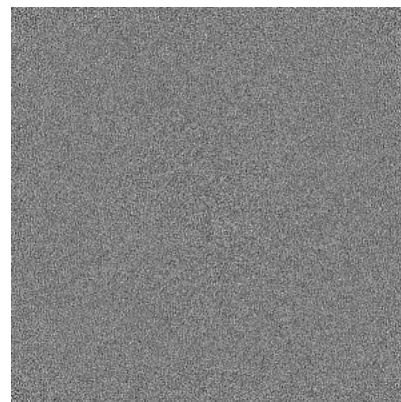
6.2.2 Raw map



X Index: 192



Y Index: 192

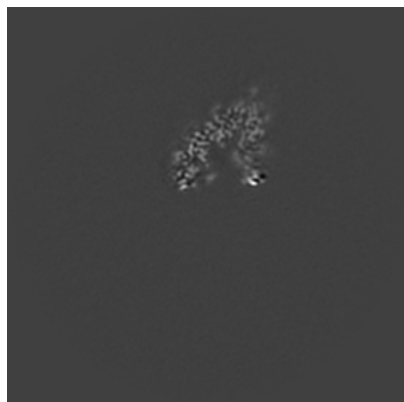


Z Index: 192

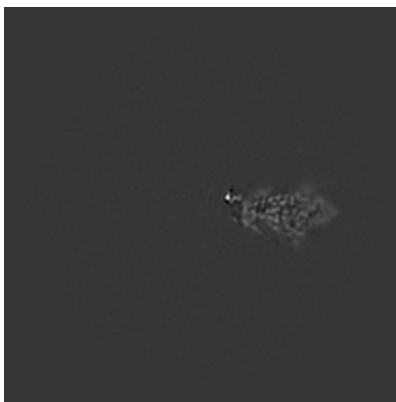
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

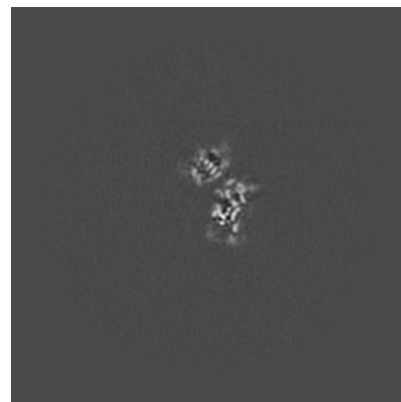
6.3.1 Primary map



X Index: 200

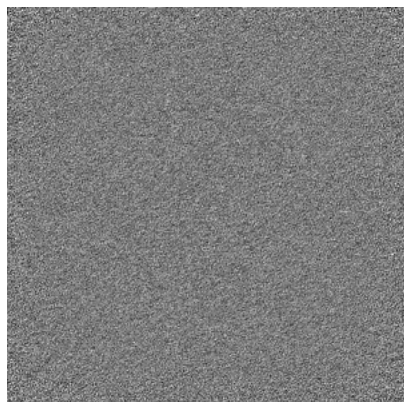


Y Index: 236

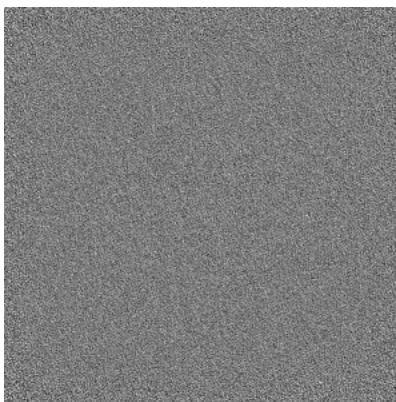


Z Index: 252

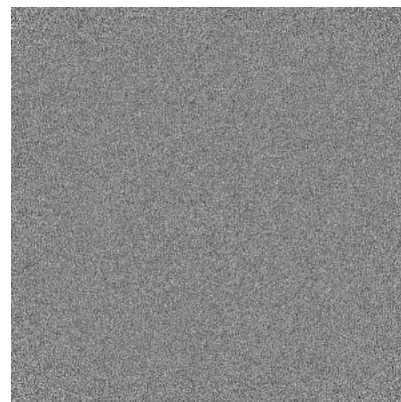
6.3.2 Raw map



X Index: 0



Y Index: 0

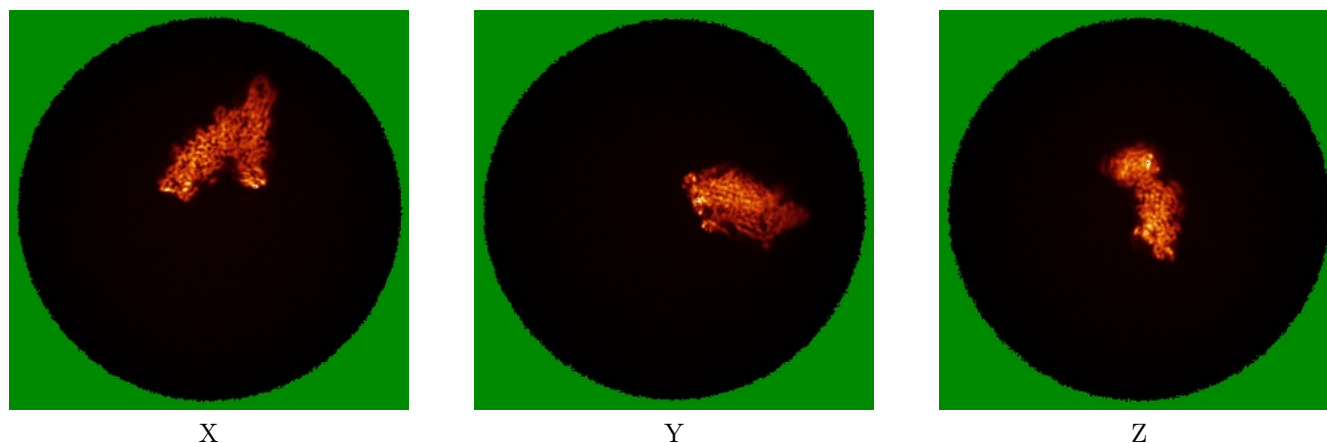


Z Index: 0

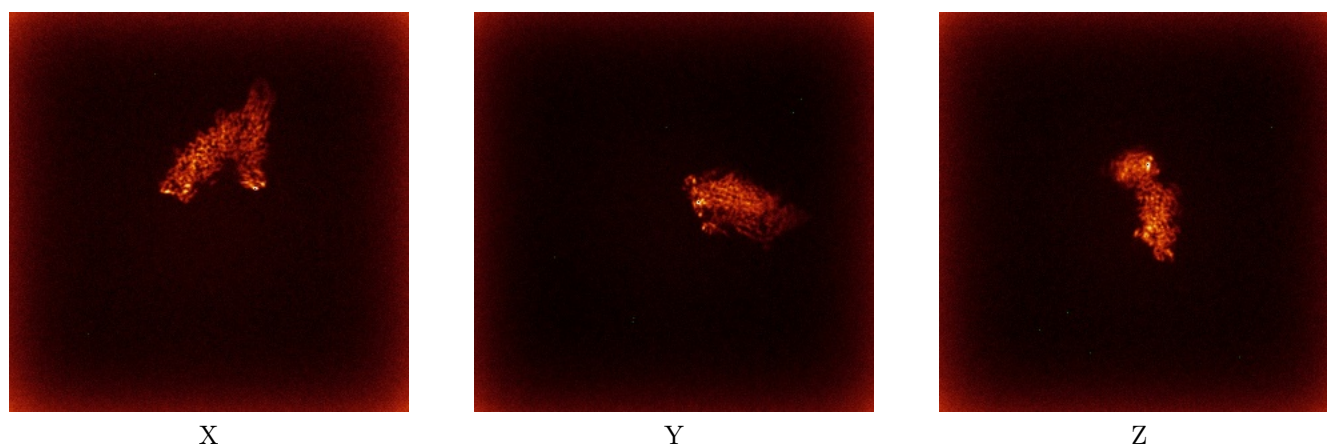
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

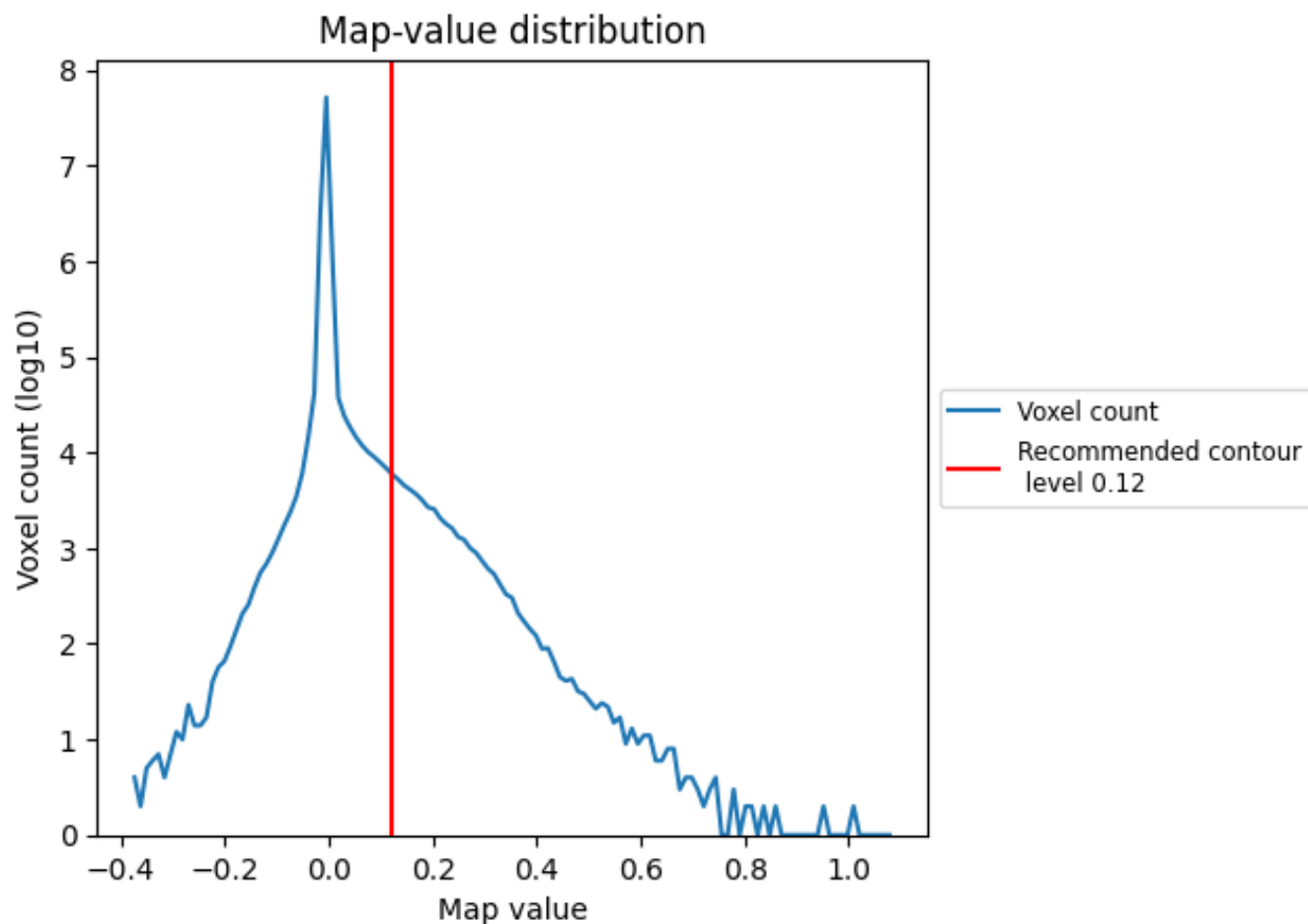
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

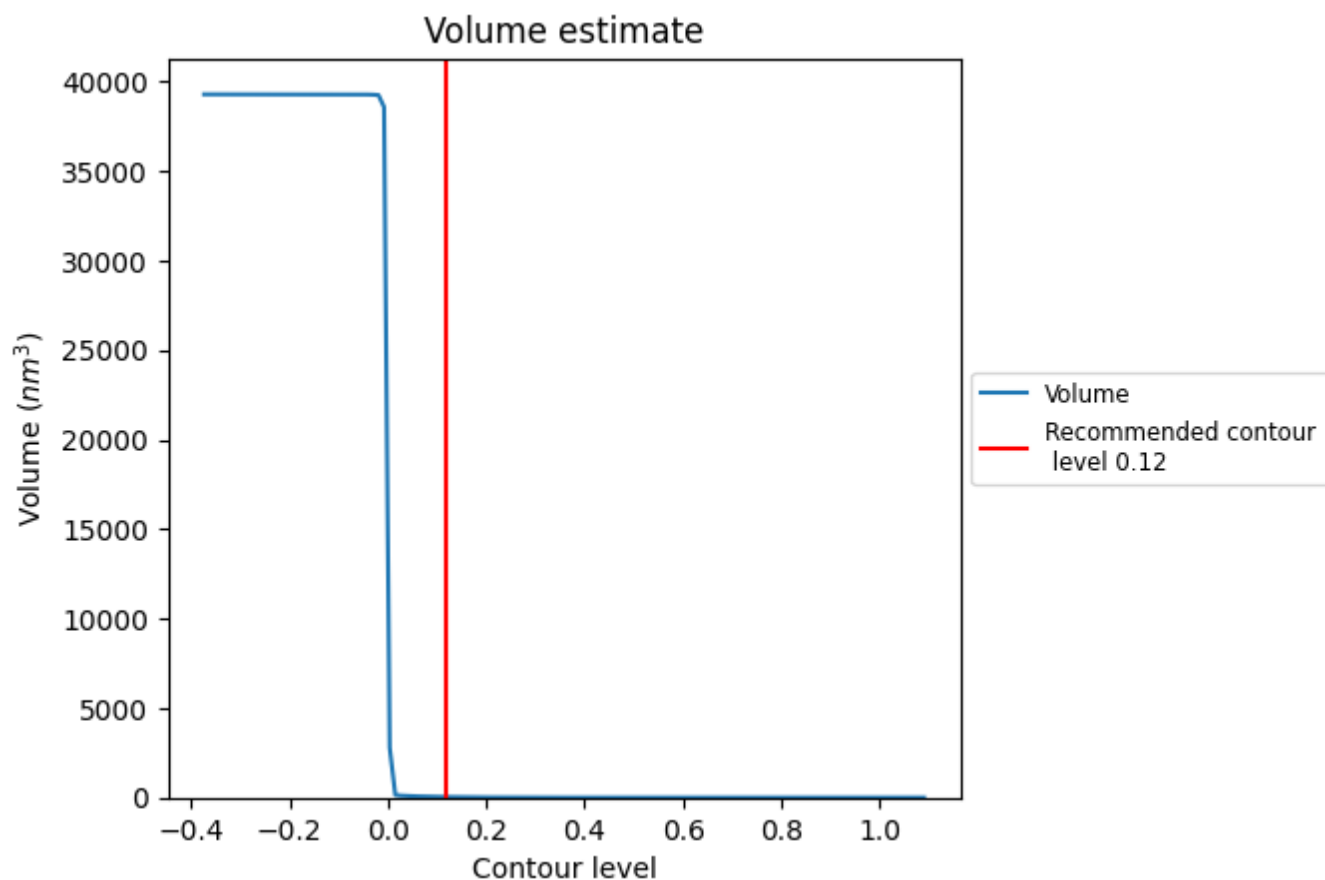
This section contains the results of statistical analysis of the map.

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.

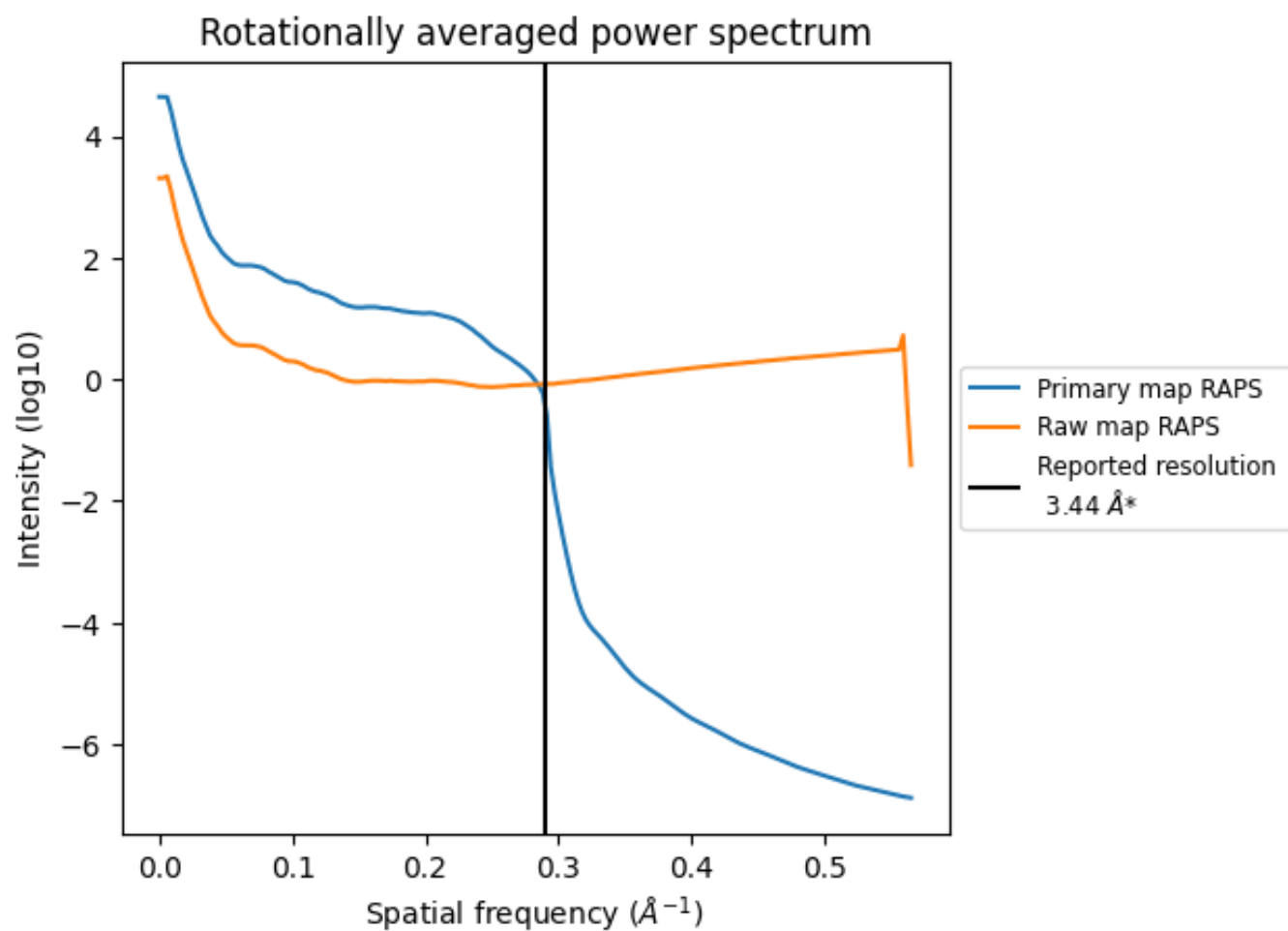
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm^3 ; this corresponds to an approximate mass of 30 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 ⓘ

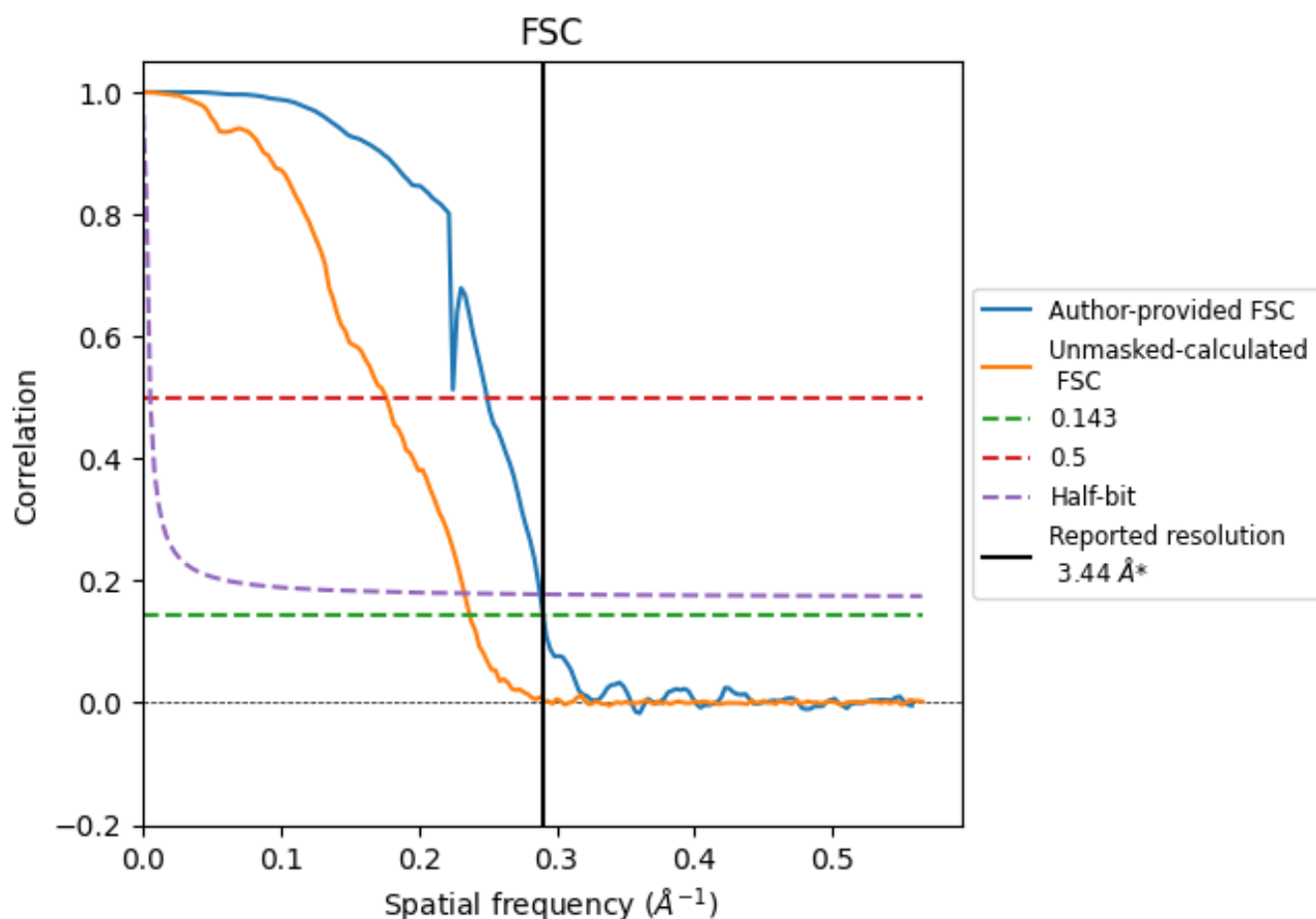


*Reported resolution corresponds to spatial frequency of $0.291 \text{ \AA}^{-1}$

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 0.291 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.44	4.00	3.47
Unmasked-calculated*	4.22	5.66	4.28

*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 4.22 differs from the reported value 3.44 by more than 10 %

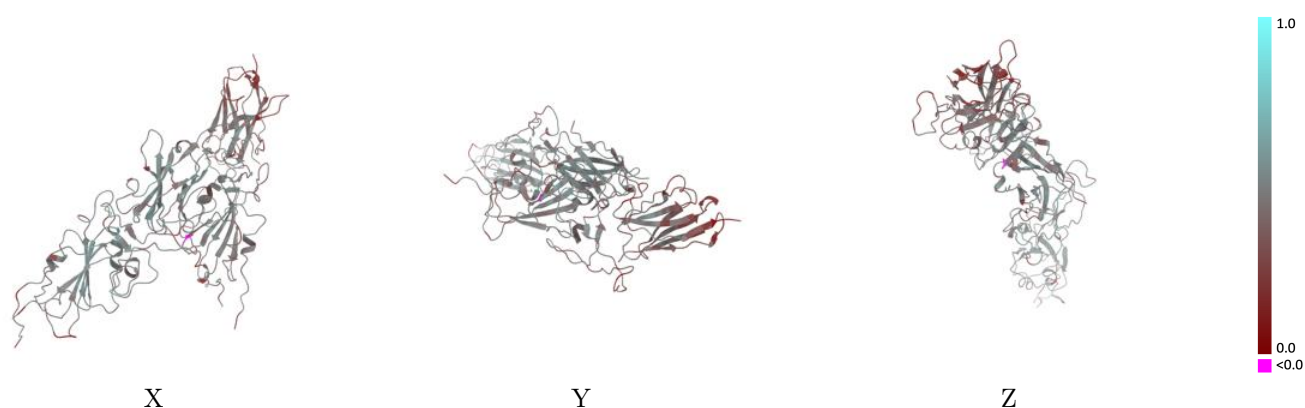
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45774 and PDB model 9CO9. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

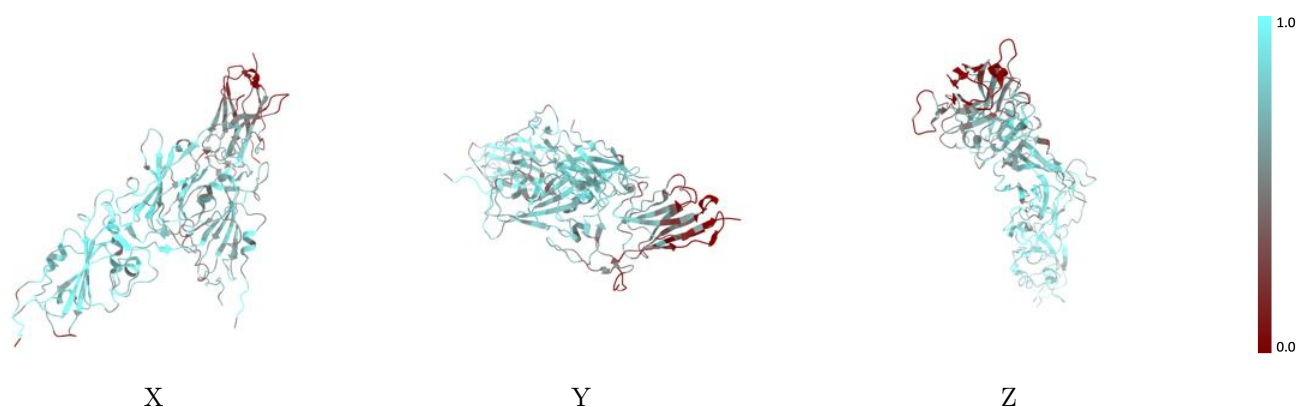
This section was not generated.

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



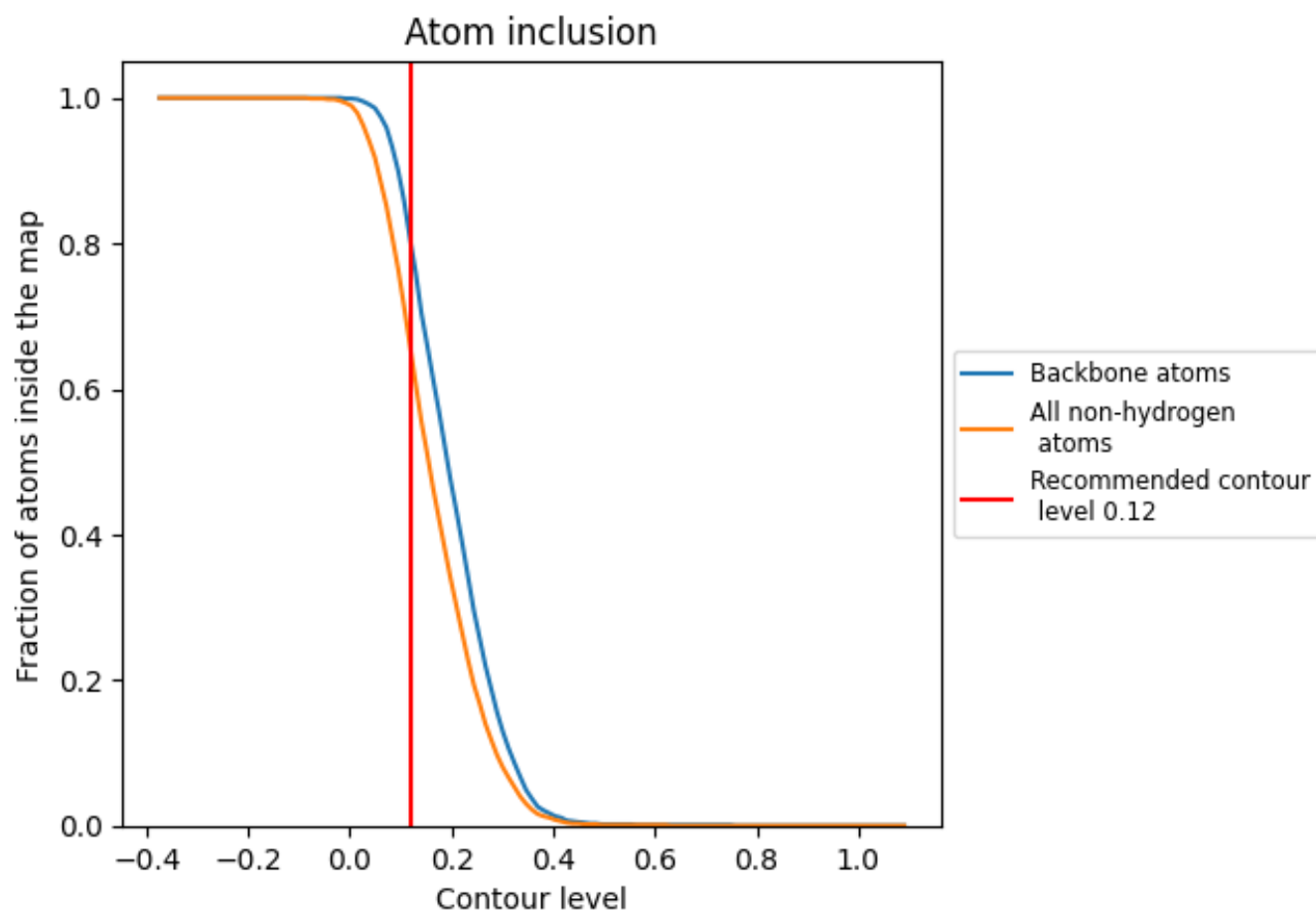
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 65% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6520	0.4380
A	0.7710	0.4680
B	0.6280	0.4320
D	0.3870	0.3560
E	0.7570	0.4770

