



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:31 AM UTC

PDB ID : 7U9P / pdb_00007u9p
EMDB ID : EMD-26404
Title : SARS-CoV-2 spike trimer RBD in complex with Fab NA8
Authors : Tsybovsky, Y.; Kwong, P.D.; Farci, P.
Deposited on : 2022-03-11
Resolution : 3.50 Å (reported)
Based on initial model : 6XLU

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
Mogul : 2022.3.0, CSD as543be (2022)
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

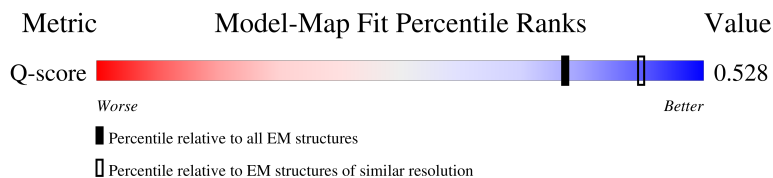
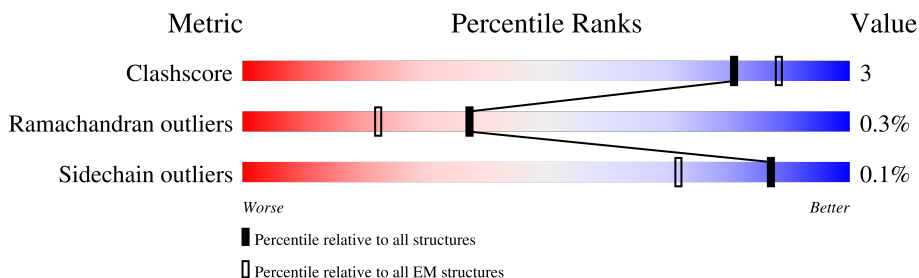
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	1275	
1	B	1275	
2	H	229	
3	L	214	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6126 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	268	Total	C	N	O	S	0	0
			2116	1351	354	401	10		
1	B	184	Total	C	N	O	S	0	0
			1507	996	239	271	1		

There are 178 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	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	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	TYR	-	expression tag	UNP P0DTC2
B	1213	ILE	-	expression tag	UNP P0DTC2
B	1214	PRO	-	expression tag	UNP P0DTC2
B	1215	GLU	-	expression tag	UNP P0DTC2
B	1216	ALA	-	expression tag	UNP P0DTC2
B	1217	PRO	-	expression tag	UNP P0DTC2
B	1218	ARG	-	expression tag	UNP P0DTC2
B	1219	ASP	-	expression tag	UNP P0DTC2
B	1220	GLY	-	expression tag	UNP P0DTC2

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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 NA8 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	168	Total	C	N	O	S	0	0
			1274	802	217	247	8		

- Molecule 3 is a protein called NA8 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	153	Total	C	N	O	S	0	0
			1173	739	191	239	4		

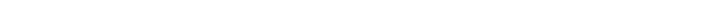
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

[illegible]

- Molecule 1: Spike glycoprotein

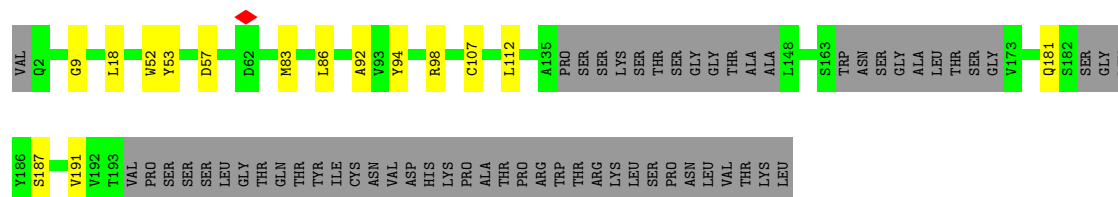
Chain B:  13% . 86%

LEU	THR	GLY	CYS	THR	THR	THR	LYS	GLN	SER	LYS	PHE	ARG	CYS	GLN
THR	VAL	PHE	MET	THR	ASN	VAL	PHE	PRO	ASN	CYS	ARG	D215	GLU	CYS
LEU	LEU	ASN	TYR	PRO	SER	VAL	LEU	ASN	ASN	TYR	VAL	G219	GLN	PHE
PRO	PRO	PHE	ILE	GLY	GLY	VAL	PHE	GLY	ASP	VAL	PRO	N234	PHE	LEU
LEU	LEU	SER	CYS	SER	SER	ALA	GLN	VAL	SER	SER	THR	ARG	CYS	THR
LEU	LEU	GLN	GLY	ALA	ALA	ILE	GLN	GLY	LYS	PRO	GLU	R237	ASN	ARG
LEU	LEU	ILE	ASP	SER	SER	HIS	PHE	TYR	VAL	THR	SER	A243	ASP	THR
GLU	GLU	PRO	THR	VAL	VAL	ASP	GLY	GLY	GLY	LEU	VAL	F140	F140	GLN
ASP	ASP	PRO	THR	VAL	VAL	ASP	PRO	PRO	GLY	LEU	ARG	L141	GLY	LEU
GLU	ASP	PRO	CYS	SER	SER	ILE	ASP	ARG	TYR	ASN	PHE	HIS	GLY	PRO
ILE	ILE	SER	SER	GLN	GLN	THR	ALA	VAL	ASN	LEU	PRO	ARG	VAL	PRO
LYS	THR	LYS	LEU	ALA	ALA	THR	VAL	PHE	ASN	VAL	THR	THR	HIS	LYS
SER	SER	ARG	GLN	THR	THR	TYR	VAL	GLU	LEU	VAL	LEU	PRO	ASN	ASN
ALA	ALA	SER	TYR	THR	THR	THR	VAL	GLY	PHE	TYR	CYS	GLY	ASN	ASN
SER	THR	THR	MET	THR	THR	THR	ARG	LEU	ARG	ALA	PRO	ASP	LYS	LYS
LEU	LEU	ILE	GLY	VAL	SER	THR	ASP	LEU	LYS	PHE	PHE	SER	SER	ILE
ALA	ALA	GLU	PHE	VAL	LEU	THR	PRO	HIS	SER	GLY	GLU	SER	THR	HIS
GLY	GLY	THR	CYS	GLY	GLY	ASN	GLN	ALA	ASN	PHE	GLU	SER	MET	VAL
THR	THR	LEU	THR	THR	GLU	VAL	LEU	PRO	LEU	VAL	PHE	GLY	GLU	SER
ILE	ILE	LEU	GLN	THR	ASN	VAL	LEU	ALA	LYS	ILE	PHE	TRP	S165	GLY
THR	THR	PHE	LEU	ASN	THR	PHE	GLU	THR	PRO	ARG	ASN	THR	V159	ASN
SER	SER	ASN	ASN	SER	SER	GLN	ILE	VAL	PHE	GLY	ALA	ALA	Y160	GLY
GLY	GLY	LYS	ARG	VAL	VAL	THR	LEU	CYS	GLU	ASP	THR	GLY	S161	THR
TRP	TRP	VAL	ALA	ALA	ALA	THR	ILE	GLY	ARG	GLY	ALA	ALA	SER	LYS
THR	THR	THR	ALA	TYR	THR	ALA	ALA	ASP	ASP	VAL	PHE	ALA	ALA	THR
LEU	LEU	LEU	THR	SER	SER	GLY	PHE	PRO	ILE	ARG	ALA	ALA	ALA	ARG
GLY	GLY	ALA	ILE	ASN	ASN	ASN	PRO	LYS	SER	GLN	SER	Y265	ASN	PHE
ALA	ALA	ASP	ILE	ASN	THR	THR	CYS	THR	THR	ILE	VAL	D287	CYS	THR
PRO	PRO	GLY	VAL	ILE	ILE	GLY	PHE	ASN	ILE	PRO	ALA	L293	T167	THR
LEU	LEU	ILE	GLN	ILE	GLU	GLY	GLY	LEU	TYR	GLY	TRP	ASN	GLN	GLY
GLN	GLN	ILE	ASP	PRO	HIS	VAL	VAL	VAL	GLN	GLN	ASN	ASP	S172	THR
ILE	ILE	LYS	LYS	THR	LYS	VAL	VAL	LYS	ALA	THR	ARG	PRO	GLN	GLY
PRO	PRO	TYR	ASN	THR	ASN	VAL	SER	ASN	GLY	LYS	ARG	SER	PHE	LEU
PHE	PHE	GLY	THR	PHE	ASN	ILE	ILE	CYS	THR	ILE	ILE	GLU	LEU	THR
PRO	PRO	ASP	GLN	THR	THR	THR	THR	VAL	PRO	ALA	SER	THR	MET	THR
MET	MET	CYS	VAL	ILE	CYS	TYR	PRO	ASN	CYS	ASP	THR	THR	LEU	ASP
GLN	GLN	THR	PHE	SER	THR	GLY	GLY	PHE	ASN	CYS	CYS	THR	GLY	LYS
ALA	ALA	ILE	GLN	THR	THR	THR	THR	ASN	GLY	VAL	THR	LEU	GLY	SER
ARG	ARG	ALA	VAL	THR	GLU	GLU	SER	ASN	GLY	ALA	ASP	LYS	GLY	THR
PHE	PHE	ALA	LYS	ILE	ILE	ILE	ASN	ASN	PHE	THR	SER	THR	GLN	THR
GLY	GLY	ASN	GLN	LEU	LEU	GLY	GLN	THR	THR	VAL	VAL	ASN	ASN	Q115
GLY	GLY	ILE	ILE	PRO	GLY	ALA	VAL	THR	CYS	CYS	THR	THR	GLY	THR
ILE	ILE	THR	LYS	VAL	VAL	GLY	ALA	THR	CYS	THR	GLU	K187	+	L117
GLY	GLY	ILE	THR	SER	PHE	ILE	VAL	PHE	THR	THR	GLY	LYS	+	+
VAL	VAL	CYS	THR	MET	THR	CYS	LEU	VAL	PRO	GLY	SER	GLY	GLY	N121
THR	THR	ALA	PRO	THR	THR	TYR	TYR	VAL	LEU	ALA	ALA	GLY	F194	ASN
GLN	GLN	GLN	PRO	LYS	THR	SER	GLN	THR	GLN	VAL	SER	ILE	I203	ALA
ASN	ASN	PHE	ILE	THR	THR	THR	ASP	GLU	SER	ILE	PHE	TYR	+	THR
VAL	VAL	THR	LYS	SER	THR	GLN	VAL	SER	TYR	ALA	THR	GLN	N211	N125
LEU	LEU	GLY	ASP	THR	THR	THR	ASN	SER	THR	THR	THR	THR	+	+
THR	THR	THR	PHE	THR	THR	GLN	CYS	THR	THR	ASN	THR	SER	LEU	THR

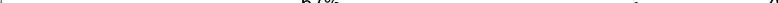
[illegible]

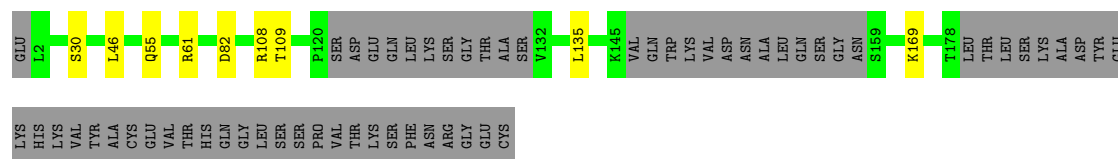
- Molecule 2: NA8 Fab heavy chain

Chain H: 67% 7% 27%



- Molecule 3: NA8 Fab light chain

Chain L:  67% 1% 29%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	454910	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	226.98001, 226.98001, 226.98001	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.873, 0.873, 0.873	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	0.58	0/2169	0.65	1/2949 (0.0%)
1	B	0.45	0/1544	0.64	0/2091
2	H	0.56	0/1304	0.70	2/1768 (0.1%)
3	L	0.55	0/1198	0.73	1/1626 (0.1%)
All	All	0.54	0/6215	0.68	4/8434 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	169	LYS	N-CA-C	-6.08	106.50	114.04
1	A	525	CYS	CA-CB-SG	5.33	126.65	114.40
2	H	107	CYS	CA-C-N	5.07	131.22	121.54
2	H	107	CYS	C-N-CA	5.07	131.22	121.54

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	2116	0	2037	10	0
1	B	1507	0	1469	10	0
2	H	1274	0	1207	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1173	0	1140	4	0
4	A	14	0	13	0	0
4	B	42	0	39	0	0
All	All	6126	0	5905	31	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.

The worst 5 of 31 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:H:9:GLY:H	2:H:18:LEU:HD21	1.64	0.63
1:A:331:ASN:HB3	1:A:580:GLN:HE22	1.66	0.60
1:A:556:ASN:O	1:A:558:LYS:NZ	2.35	0.59
1:A:454:ARG:NH2	1:A:467:ASP:O	2.35	0.59
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.86	0.57

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	264/1275 (21%)	234 (89%)	29 (11%)	1 (0%)	30	62
1	B	164/1275 (13%)	146 (89%)	18 (11%)	0	100	100
2	H	160/229 (70%)	141 (88%)	19 (12%)	0	100	100
3	L	147/214 (69%)	127 (86%)	19 (13%)	1 (1%)	18	51
All	All	735/2993 (25%)	648 (88%)	85 (12%)	2 (0%)	37	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	30	SER
1	A	527	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/1103 (21%)	235 (100%)	1 (0%)	84	81
1	B	168/1103 (15%)	168 (100%)	0	100	100
2	H	138/189 (73%)	138 (100%)	0	100	100
3	L	136/189 (72%)	136 (100%)	0	100	100
All	All	678/2584 (26%)	677 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	524	VAL

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	196	ASN
2	H	82	GLN
2	H	181	GLN
1	A	474	GLN
1	A	409	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	1303	1	14,14,15	0.34	0	17,19,21	0.51	0
4	NAG	B	1302	1	14,14,15	0.31	0	17,19,21	0.64	1 (5%)
4	NAG	B	1301	1	14,14,15	0.72	1 (7%)	17,19,21	0.70	1 (5%)
4	NAG	A	1301	1	14,14,15	0.34	0	17,19,21	0.90	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1301	NAG	C1-C2	2.06	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	NAG	C1-O5-C5	3.06	116.28	112.19
4	B	1301	NAG	C1-O5-C5	2.23	115.17	112.19
4	B	1302	NAG	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1301	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

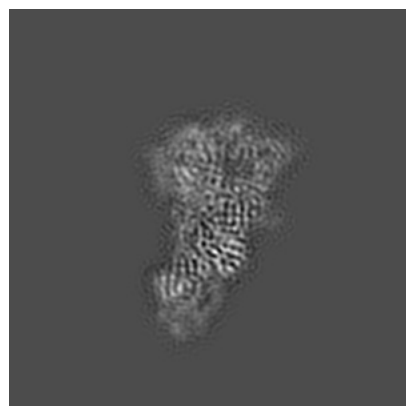
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26404. These allow visual inspection of the internal detail of the map and identification of artifacts.

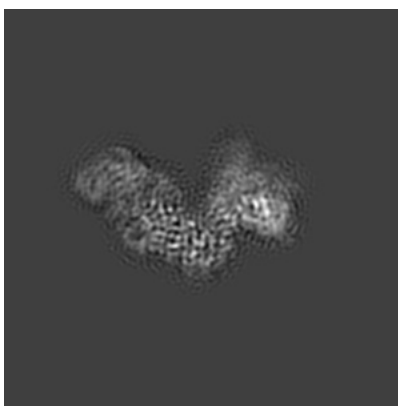
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

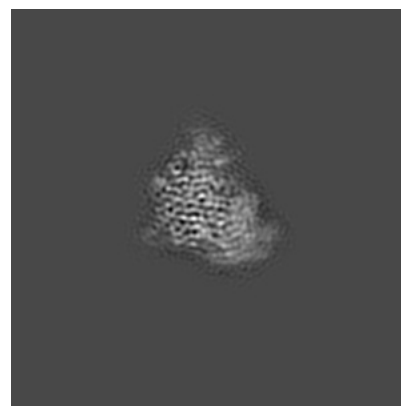
6.1.1 Primary map



X

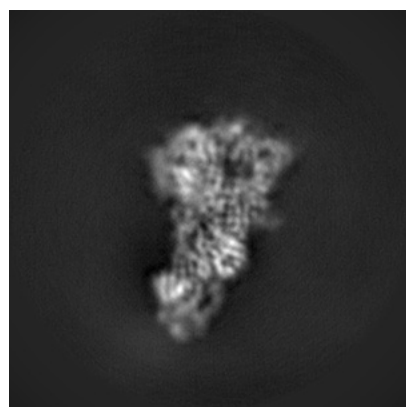


Y

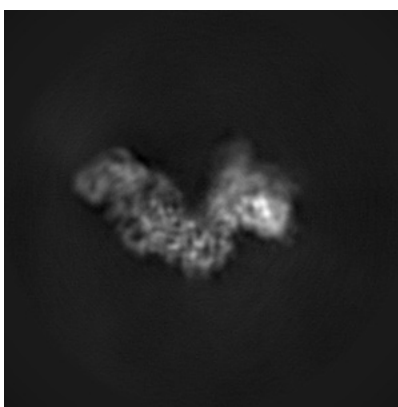


Z

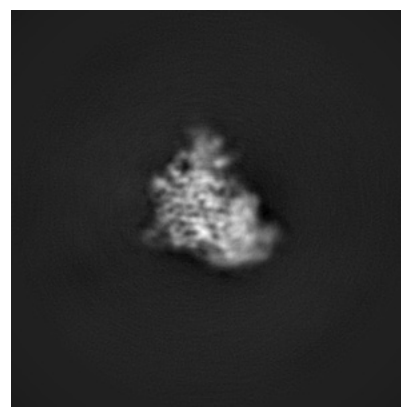
6.1.2 Raw map



X



Y

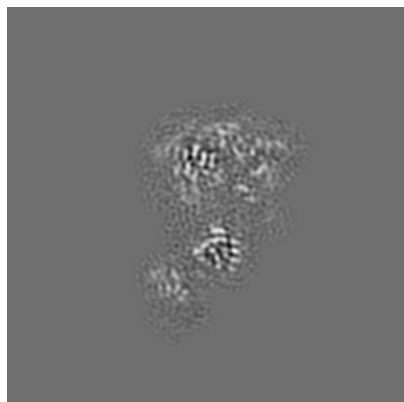


Z

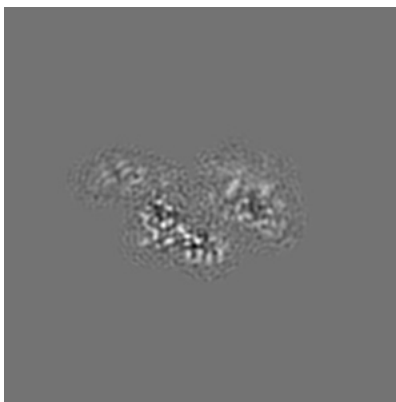
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

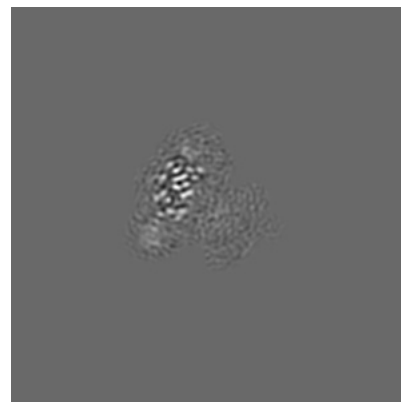
6.2.1 Primary map



X Index: 130

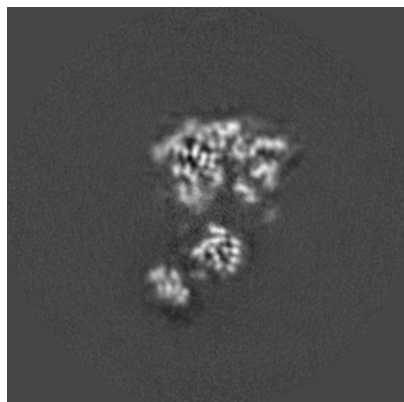


Y Index: 130

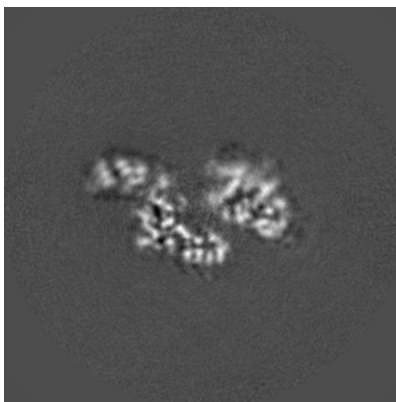


Z Index: 130

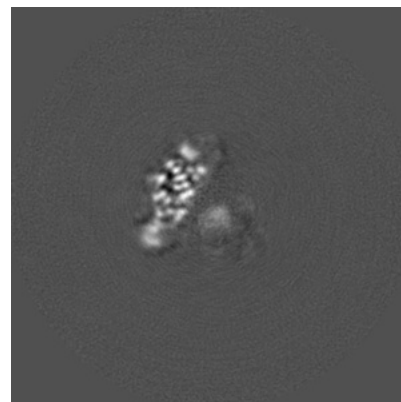
6.2.2 Raw map



X Index: 130



Y Index: 130

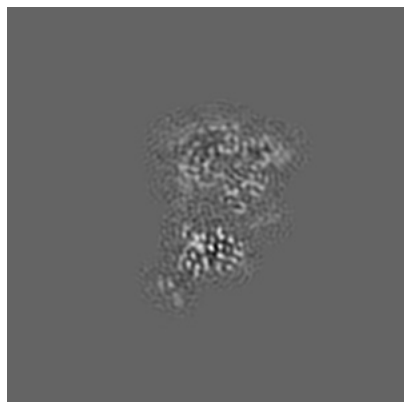


Z Index: 130

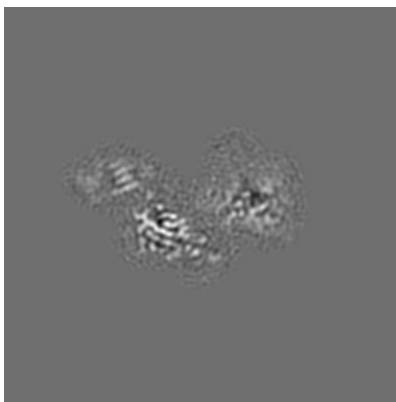
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 124

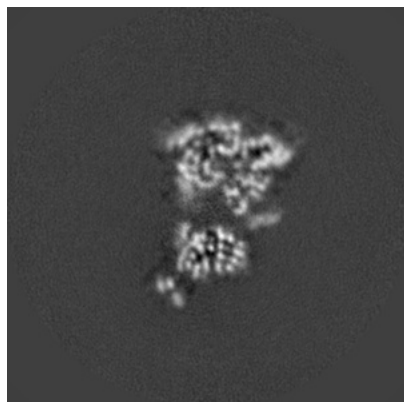


Y Index: 123

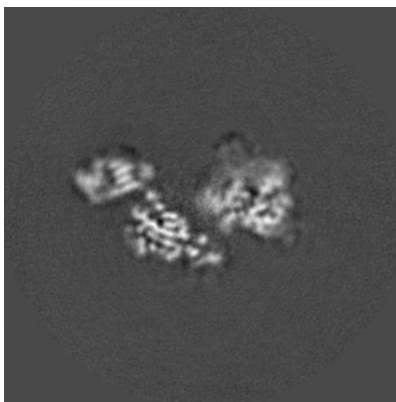


Z Index: 102

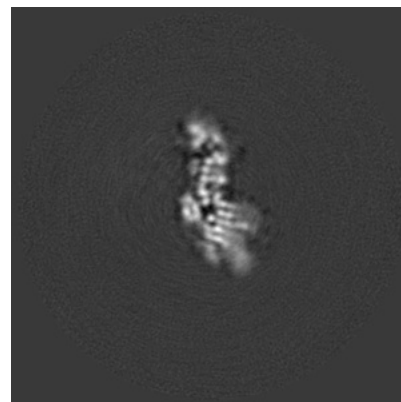
6.3.2 Raw map



X Index: 124



Y Index: 123

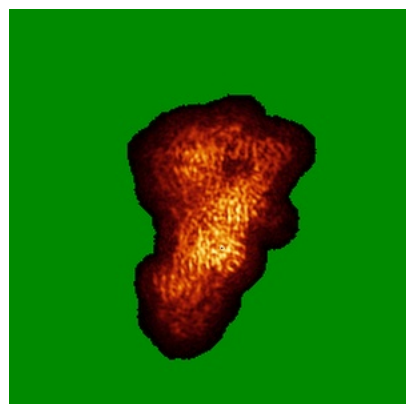


Z Index: 167

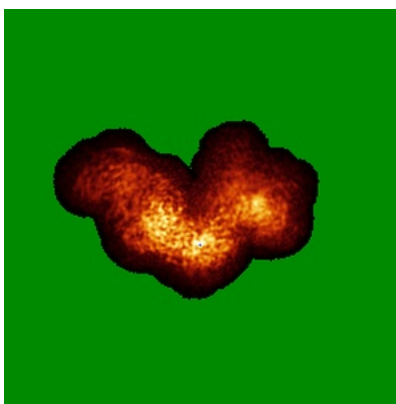
The images above show the largest variance slices of the map in three orthogonal directions.

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

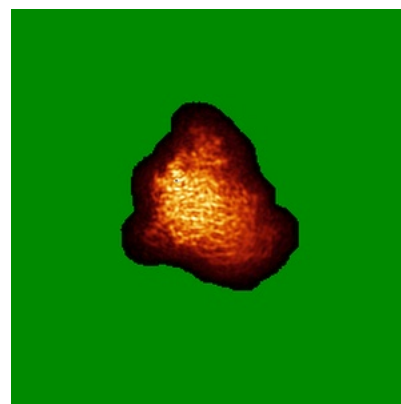
6.4.1 Primary map



X



Y



Z

6.4.2 Raw map



X



Y

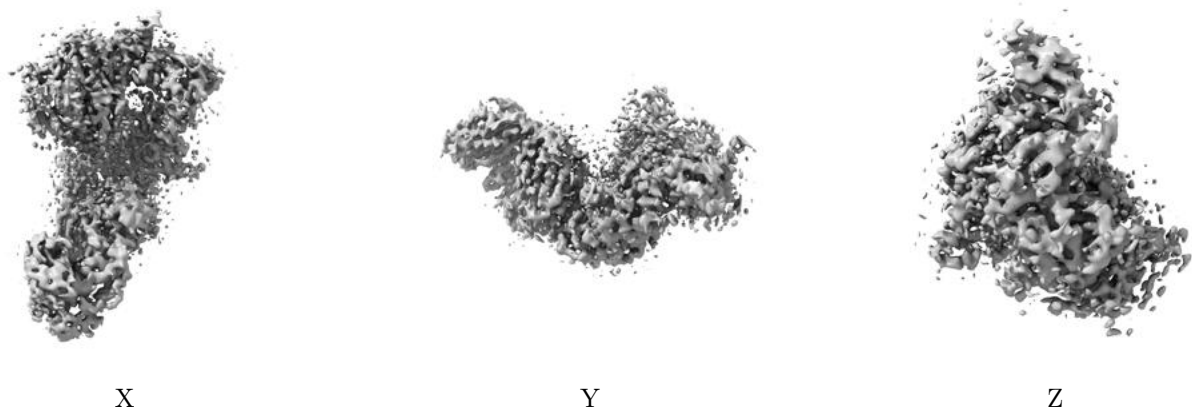


Z

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.

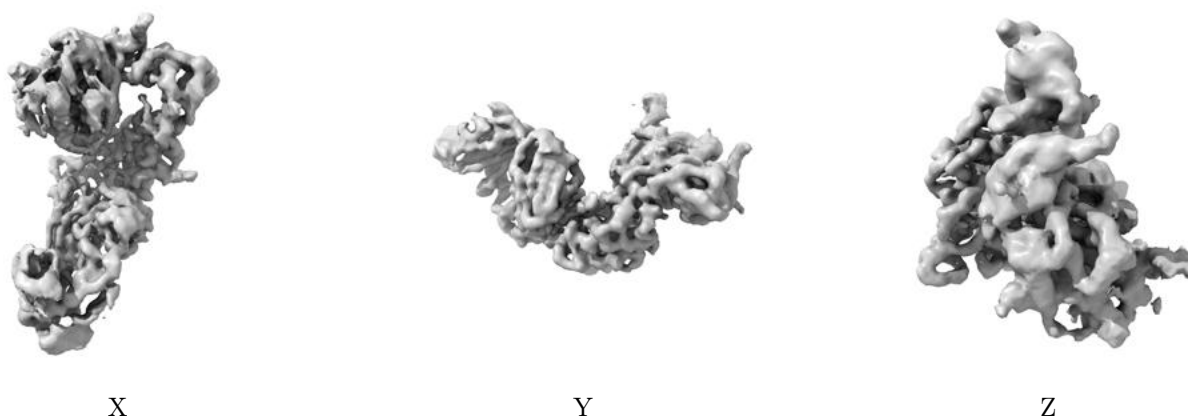
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

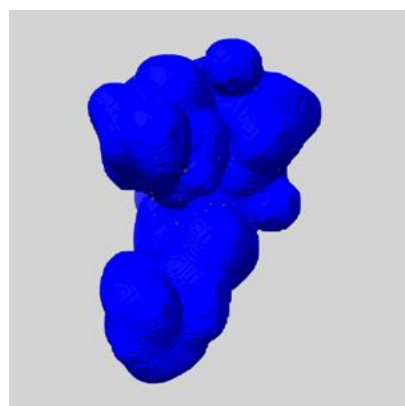
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

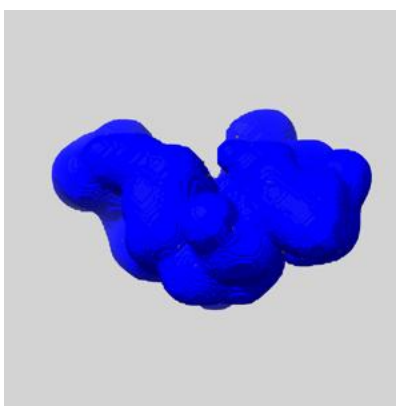
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

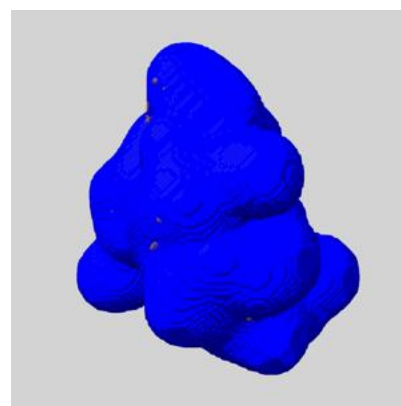
6.6.1 emd_26404_msk_1.map [i](#)



X



Y

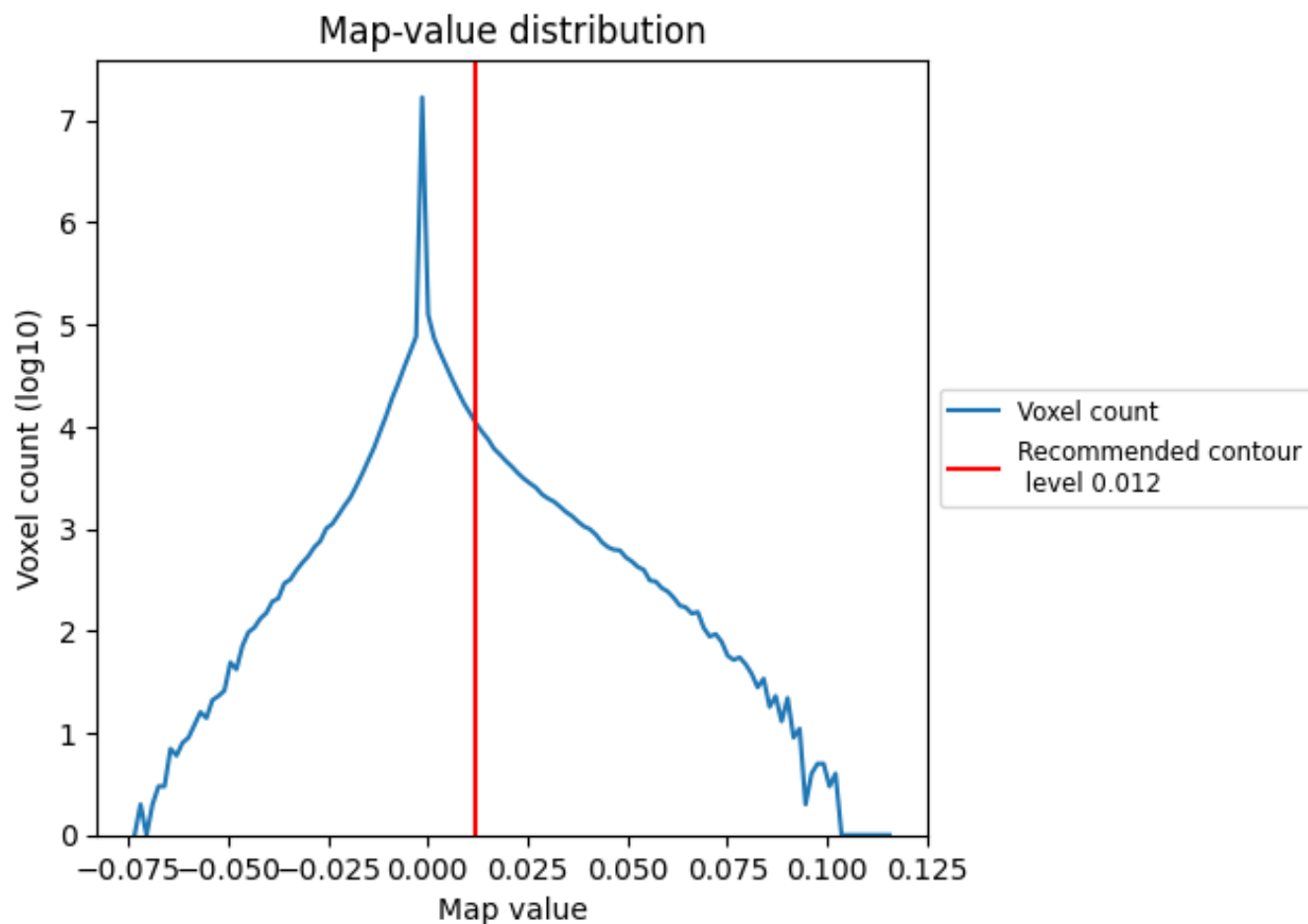


Z

7 Map analysis [i](#)

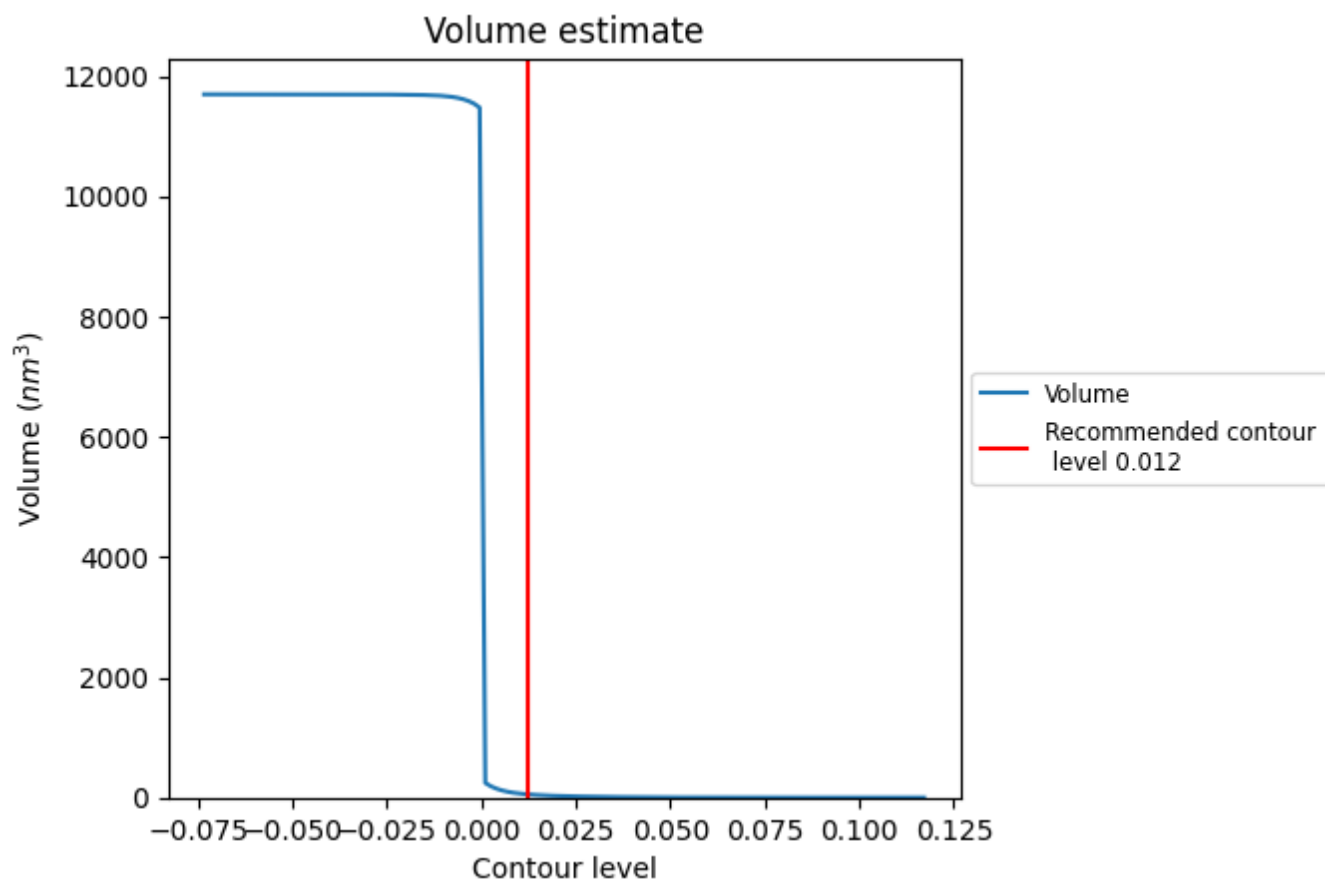
This section contains the results of statistical analysis of the map.

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.

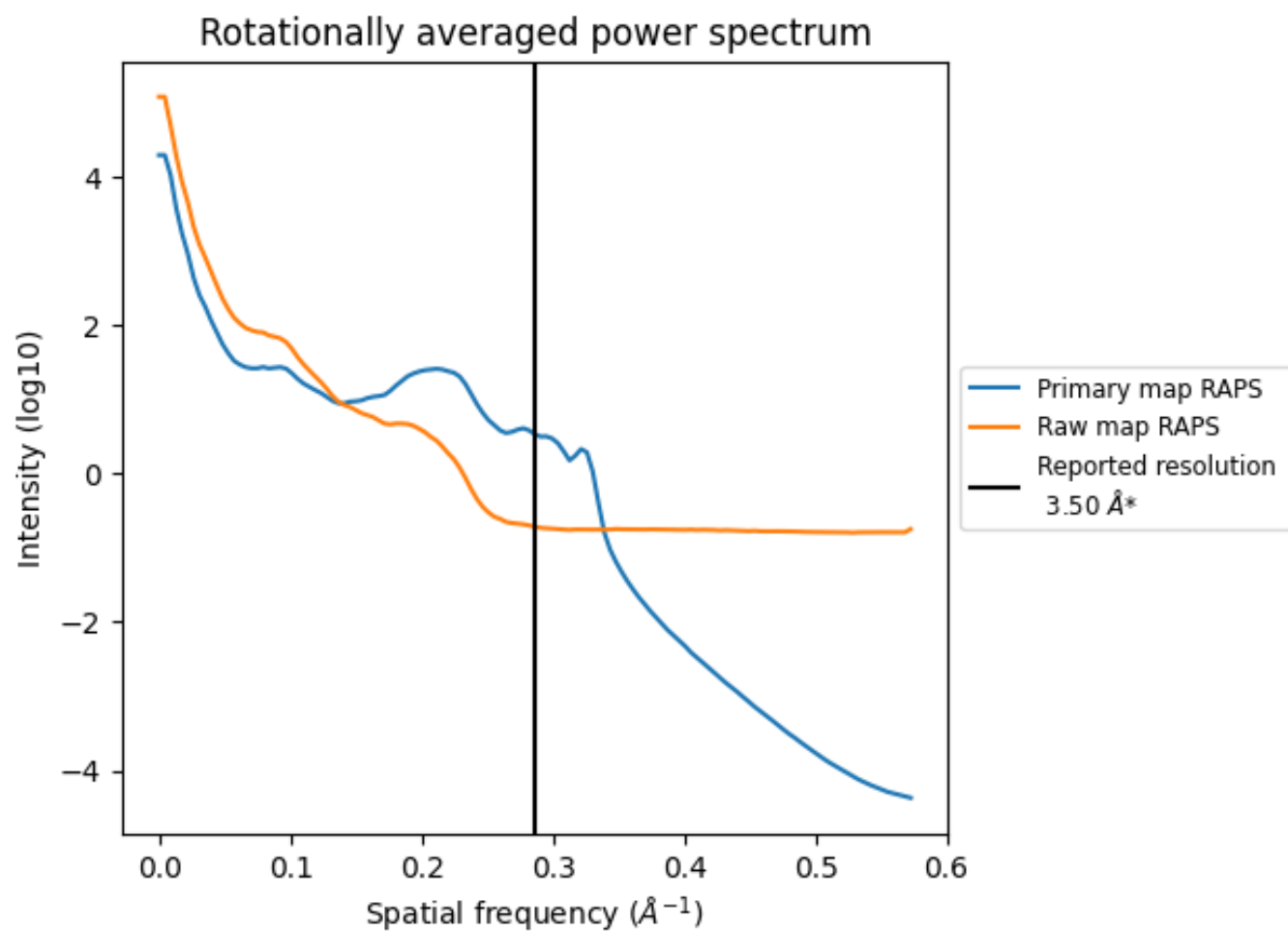
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 55 nm³; this corresponds to an approximate mass of 49 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 ⓘ

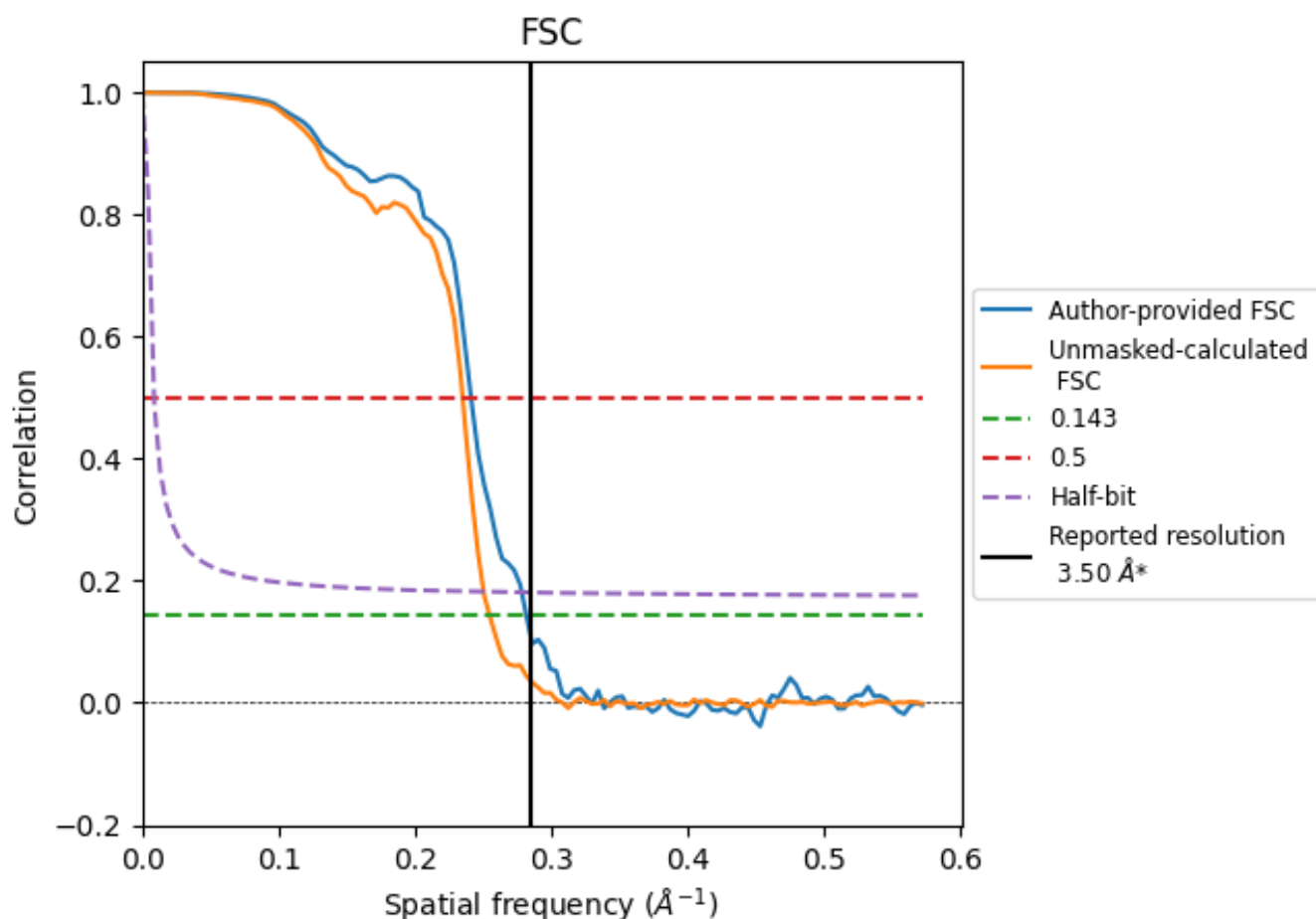


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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](#)

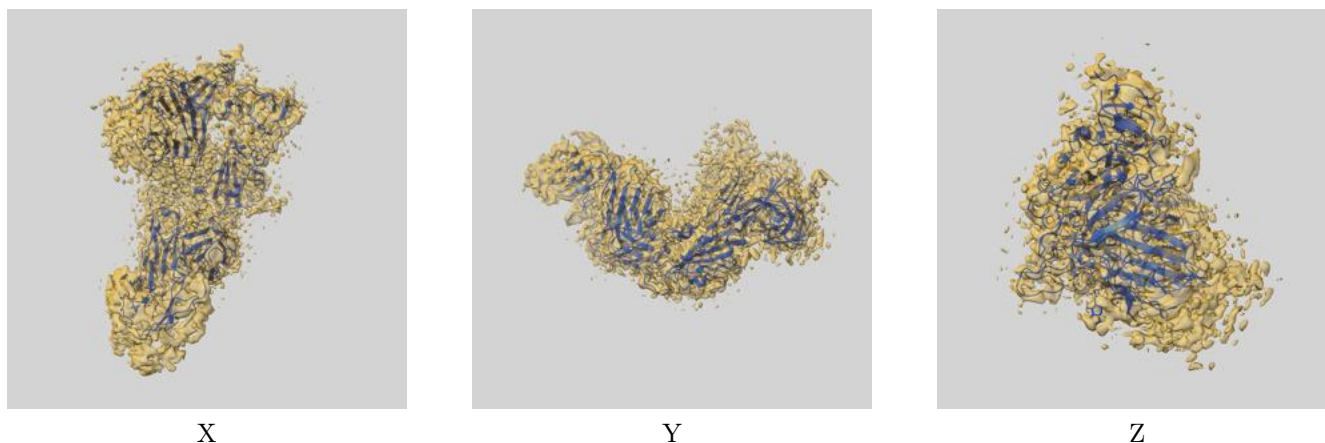
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.55	4.14	3.59
Unmasked-calculated*	3.92	4.25	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

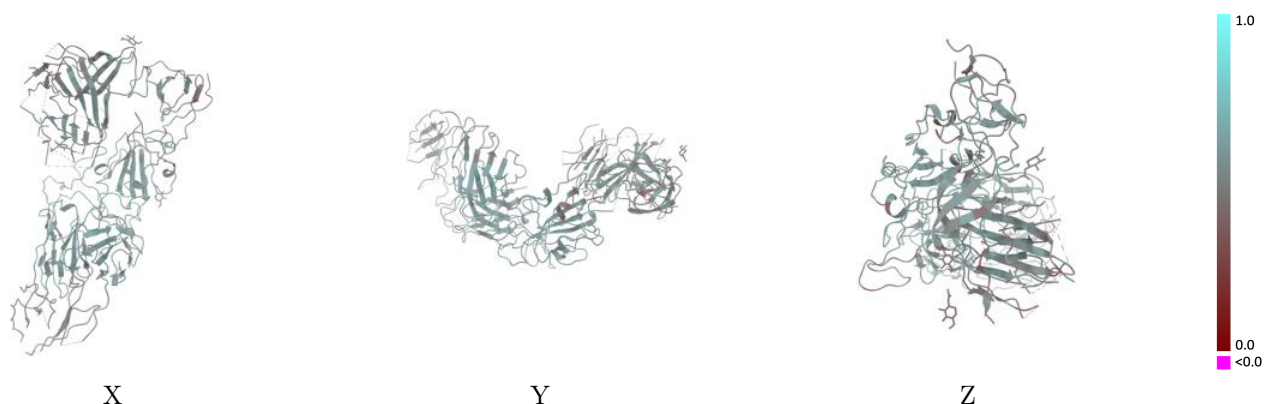
This section contains information regarding the fit between EMDB map EMD-26404 and PDB model 7U9P. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



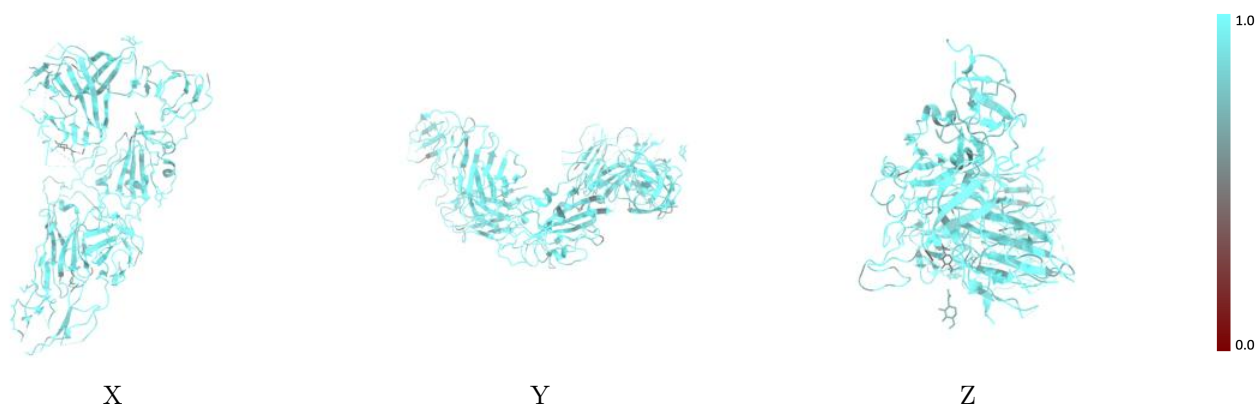
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



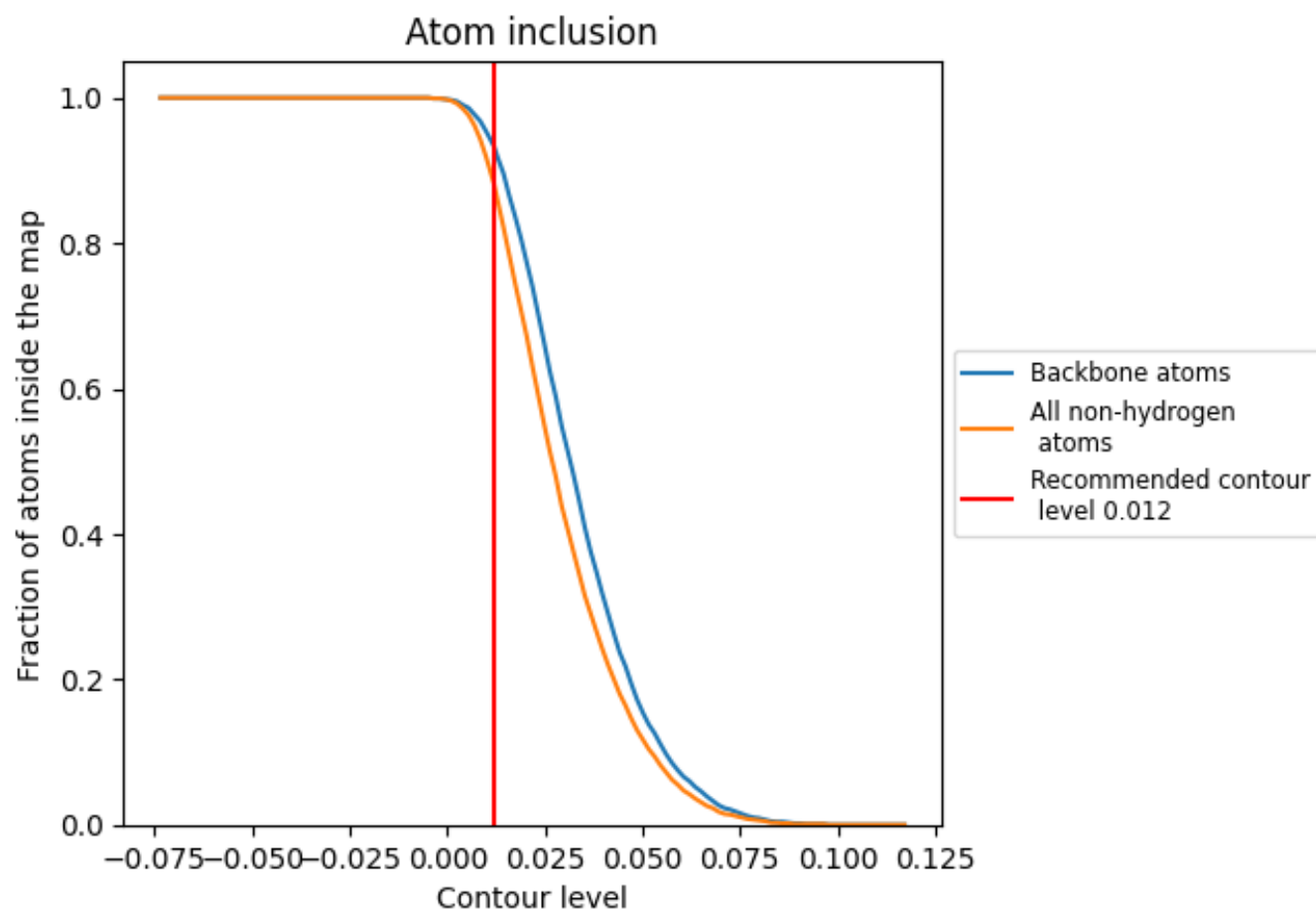
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 88% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.5280
A	0.8850	0.5320
B	0.8670	0.5000
H	0.8930	0.5500
L	0.8800	0.5360

