



## wwPDB EM Validation Summary Report ⓘ

Jun 6, 2024 – 01:25 pm BST

PDB ID : 9FGT  
EMDB ID : EMD-50424  
Title : SARS-CoV-2 (B.1.1.529/Omicron variant) Spike protein in complex with the single chain fragment scFv76 (focused refinement)  
Authors : Berlinguer, M.; Chaves-Sanjuan, A.; Milazzo, F.M.; Minenkova, O.; De Santis, R.; Bolognesi, M.  
Deposited on : 2024-05-25  
Resolution : 3.80 Å (reported)  
Based on initial model : 7zce

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>.

---

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

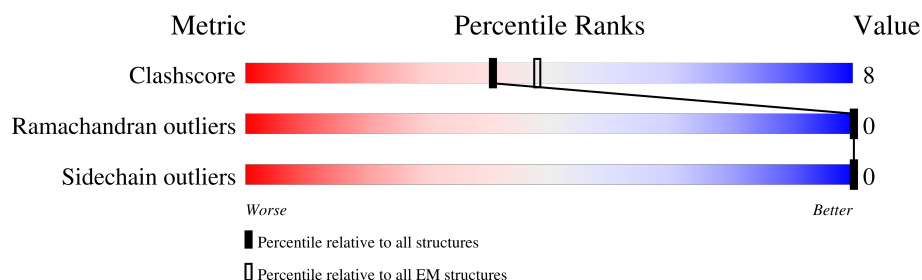
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	C	1214	 10% 87%
2	E	264	 5% 68% 14% 18%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2921 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	157	Total	C	N	O	S	0	0
			1280	828	219	229	4		

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	82	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	SER	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	84	SER	LYS	variant	UNP P0DTC2
C	102	ILE	THR	variant	UNP P0DTC2
C	149	ASP	GLY	variant	UNP P0DTC2
C	218	ILE	ASN	variant	UNP P0DTC2
C	219	VAL	LEU	variant	UNP P0DTC2
C	220	PRO	VAL	variant	UNP P0DTC2
C	221	GLU	ARG	variant	UNP P0DTC2
C	?	-	SER	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	ASP	deletion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	ILE	deletion	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	ASP	deletion	UNP P0DTC2
C	?	-	GLN	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	TRP	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	SER	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	SER	deletion	UNP P0DTC2
C	635	TYR	HIS	variant	UNP P0DTC2
C	?	-	GLN	deletion	UNP P0DTC2
C	?	-	THR	deletion	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	?	-	SER	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	732	LYS	ASN	variant	UNP P0DTC2
C	764	TYR	ASP	variant	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	ASP	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	PHE	deletion	UNP P0DTC2
C	?	-	ILE	deletion	UNP P0DTC2
C	?	-	LYS	deletion	UNP P0DTC2
C	?	-	GLN	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	ASP	deletion	UNP P0DTC2
C	?	-	CYS	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	ASP	deletion	UNP P0DTC2
C	?	-	ILE	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ASP	deletion	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ILE	deletion	UNP P0DTC2
C	?	-	CYS	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	?	-	GLN	deletion	UNP P0DTC2
C	797	LYS	ASN	variant	UNP P0DTC2
C	895	HIS	GLN	variant	UNP P0DTC2
C	910	LYS	ASN	variant	UNP P0DTC2
C	922	PHE	LEU	variant	UNP P0DTC2
C	927	PRO	LYS	engineered mutation	UNP P0DTC2
C	928	PRO	VAL	engineered mutation	UNP P0DTC2
C	1150	GLY	-	linker	UNP P0DTC2
C	1151	SER	-	linker	UNP P0DTC2
C	1173	LEU	PHE	engineered mutation	UNP P10104
C	1179	GLY	-	expression tag	UNP P10104

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	1180	ARG	-	expression tag	UNP P10104
C	1181	SER	-	expression tag	UNP P10104
C	1182	LEU	-	expression tag	UNP P10104
C	1183	GLU	-	expression tag	UNP P10104
C	1184	VAL	-	expression tag	UNP P10104
C	1185	LEU	-	expression tag	UNP P10104
C	1186	PHE	-	expression tag	UNP P10104
C	1187	GLN	-	expression tag	UNP P10104
C	1188	GLY	-	expression tag	UNP P10104
C	1189	PRO	-	expression tag	UNP P10104
C	1190	GLY	-	expression tag	UNP P10104
C	1191	HIS	-	expression tag	UNP P10104
C	1192	HIS	-	expression tag	UNP P10104
C	1193	HIS	-	expression tag	UNP P10104
C	1194	HIS	-	expression tag	UNP P10104
C	1195	HIS	-	expression tag	UNP P10104
C	1196	HIS	-	expression tag	UNP P10104
C	1197	HIS	-	expression tag	UNP P10104
C	1198	HIS	-	expression tag	UNP P10104
C	1199	SER	-	expression tag	UNP P10104
C	1200	ALA	-	expression tag	UNP P10104
C	1201	TRP	-	expression tag	UNP P10104
C	1202	SER	-	expression tag	UNP P10104
C	1203	HIS	-	expression tag	UNP P10104
C	1204	PRO	-	expression tag	UNP P10104
C	1205	GLN	-	expression tag	UNP P10104
C	1206	PHE	-	expression tag	UNP P10104
C	1207	GLU	-	expression tag	UNP P10104
C	1208	LYS	-	expression tag	UNP P10104
C	1209	GLY	-	expression tag	UNP P10104
C	1210	GLY	-	expression tag	UNP P10104
C	1211	GLY	-	expression tag	UNP P10104
C	1212	SER	-	expression tag	UNP P10104
C	1213	GLY	-	expression tag	UNP P10104
C	1214	GLY	-	expression tag	UNP P10104
C	1215	GLY	-	expression tag	UNP P10104
C	1216	GLY	-	expression tag	UNP P10104
C	1217	SER	-	expression tag	UNP P10104
C	1218	GLY	-	expression tag	UNP P10104
C	1219	GLY	-	expression tag	UNP P10104
C	1220	SER	-	expression tag	UNP P10104
C	1221	ALA	-	expression tag	UNP P10104

*Continued on next page...*

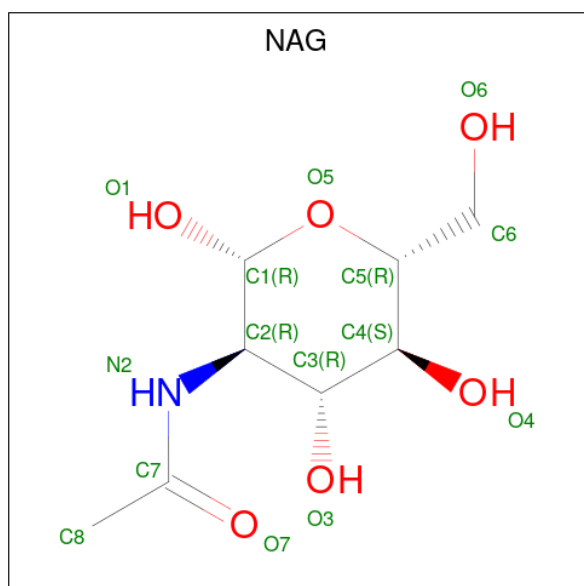
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1222	TRP	-	expression tag	UNP P10104
C	1223	SER	-	expression tag	UNP P10104
C	1224	HIS	-	expression tag	UNP P10104
C	1225	PRO	-	expression tag	UNP P10104
C	1226	GLN	-	expression tag	UNP P10104
C	1227	PHE	-	expression tag	UNP P10104
C	1228	GLU	-	expression tag	UNP P10104
C	1229	LYS	-	expression tag	UNP P10104

- Molecule 2 is a protein called Single chain fragment scFv76.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	216	Total	C	N	O	S	0	0
			1627	1027	276	318	6		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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





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

● Molecule 2: Single chain fragment scFv76



GLY	ASP	GLY	ARG
TYR	THR	GLY	THR
LYS	MET	SER	MET
ASP	GLU	GLU	GLU
ASP	E1	V2	E1
ASP	Q3	Q3	V2
ASP	Q3	Q3	Q3
ASP	L4	L4	L4
LYS	S17	S17	S17
HIS	C22	C22	C22
HIS	G26	G26	G26
HIS	F27	F27	F27
HIS	S30	S30	S30
HIS	A31	A31	A31
HIS	N32	N32	N32
HIS	K43	K43	K43
HIS	W47	W47	W47
HIS	V50	V50	V50
HIS	P53	P53	P53
HIS	F58	F58	F58
HIS	K64	K64	K64
HIS	R71	R71	R71
HIS	M82	M82	M82
HIS	L85	L85	L85
HIS	R97	R97	R97
HIS	S100	S100	S100
HIS	G103	G103	G103
HIS	L113	L113	L113
HIS	S117	S117	S117
HIS	SER	SER	SER
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS	GLY	GLY	GLY
HIS			

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	7538	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.505	Depositor
Minimum map value	-3.289	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.7	Depositor
Map size ( $\text{\AA}$ )	355.6, 355.6, 355.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.889, 0.889, 0.889	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	C	0.36	0/1317	0.54	0/1783
2	E	0.34	0/1662	0.55	0/2256
All	All	0.35	0/2979	0.54	0/4039

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1280	0	1218	21	0
2	E	1627	0	1582	25	0
3	C	14	0	13	0	0
All	All	2921	0	2813	43	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 8.

The worst 5 of 43 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:E:32:ASN:HD22	2:E:97:ARG:HH21	1.28	0.79
2:E:2:VAL:HG12	2:E:26:GLY:HA3	1.70	0.73
2:E:139:GLN:NE2	2:E:222:CYS:SG	2.64	0.71
1:C:421:TYR:OH	2:E:53:PRO:O	2.09	0.69
1:C:409:GLN:HB3	1:C:419:ALA:HB2	1.74	0.68

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	C	151/1214 (12%)	141 (93%)	10 (7%)	0	100	100
2	E	210/264 (80%)	192 (91%)	18 (9%)	0	100	100
All	All	361/1478 (24%)	333 (92%)	28 (8%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	136/1059 (13%)	136 (100%)	0	100	100
2	E	175/207 (84%)	175 (100%)	0	100	100
All	All	311/1266 (25%)	311 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	C	1301	1	14,14,15	0.94	1 (7%)	17,19,21	1.65	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
3	NAG	C	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)
3	C	1301	NAG	O5-C1	3.38	1.49	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	C	1301	NAG	C1-O5-C5	6.33	120.77	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1301	NAG	C3-C2-N2-C7
3	C	1301	NAG	C1-C2-N2-C7

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.

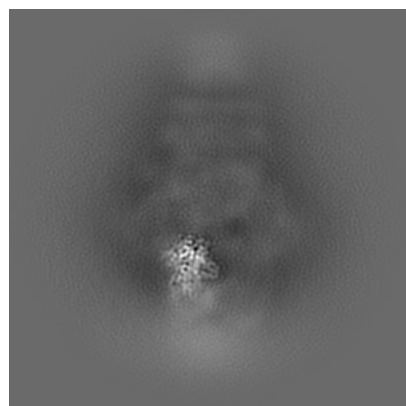
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50424. These allow visual inspection of the internal detail of the map and identification of artifacts.

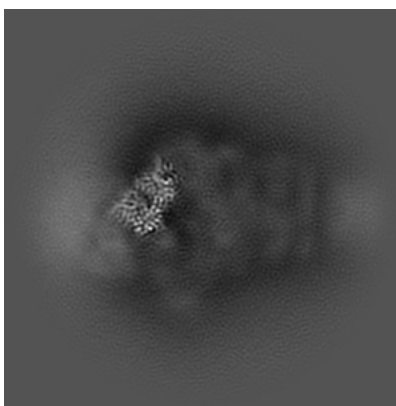
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

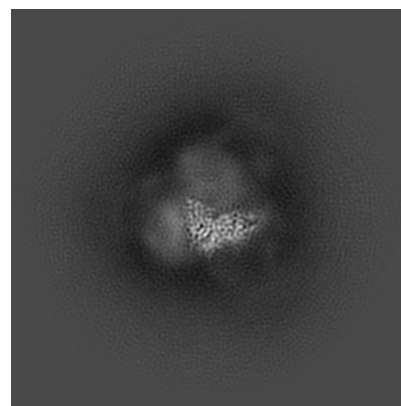
#### 6.1.1 Primary map



X

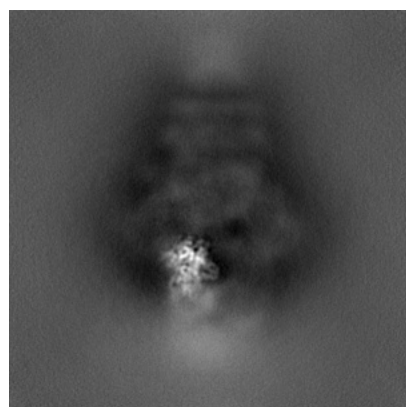


Y

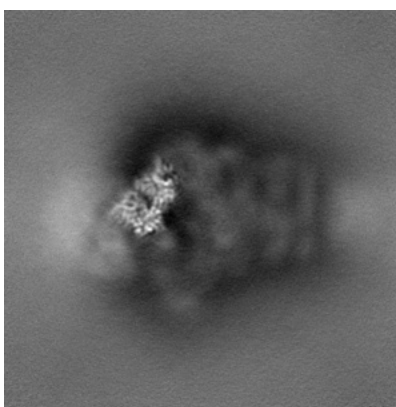


Z

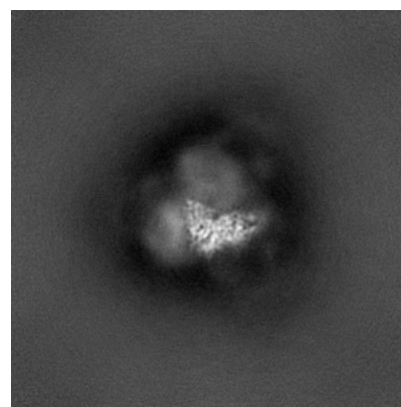
#### 6.1.2 Raw map



X



Y

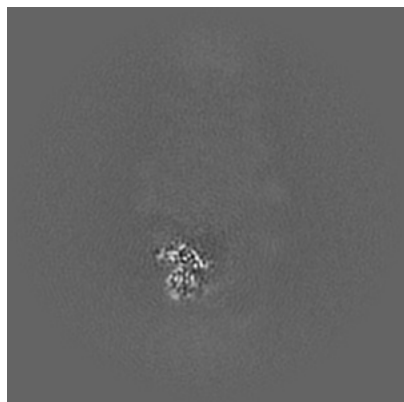


Z

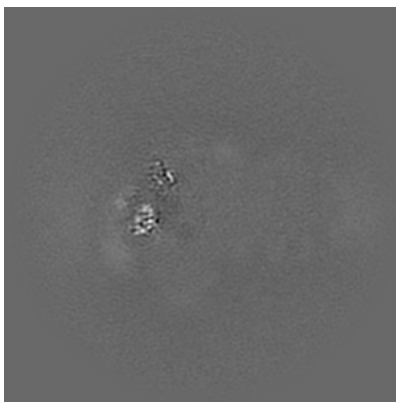
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

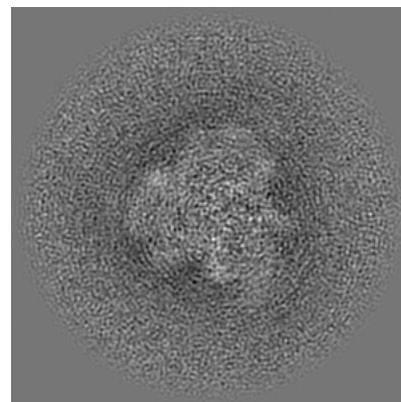
### 6.2.1 Primary map



X Index: 200

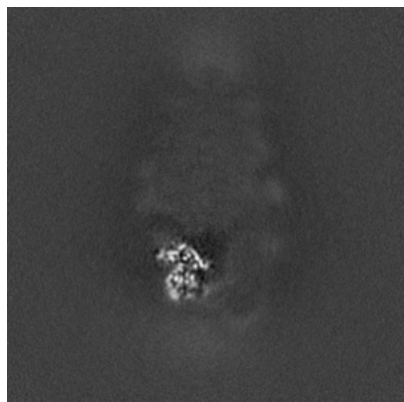


Y Index: 200

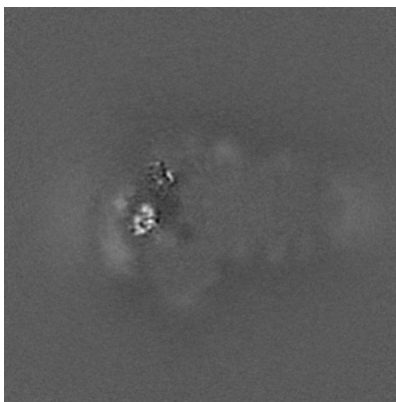


Z Index: 200

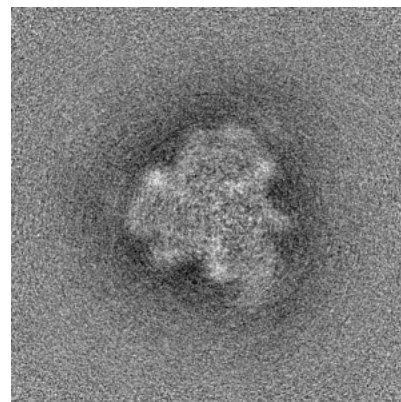
### 6.2.2 Raw map



X Index: 200



Y Index: 200



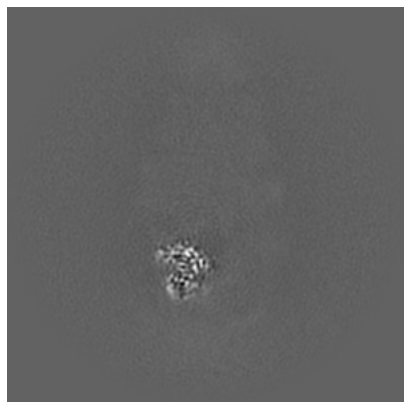
Z Index: 200

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

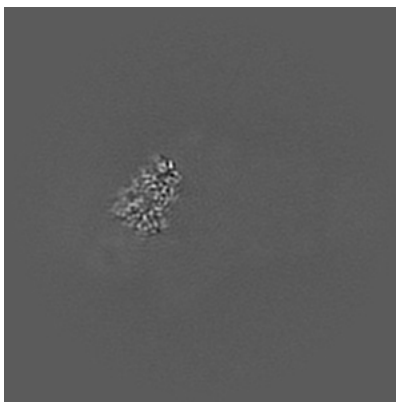


## 6.3 Largest variance slices [i](#)

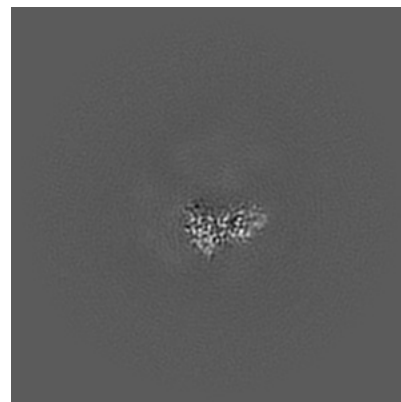
### 6.3.1 Primary map



X Index: 198

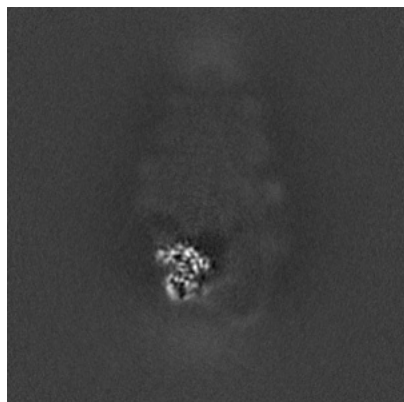


Y Index: 180

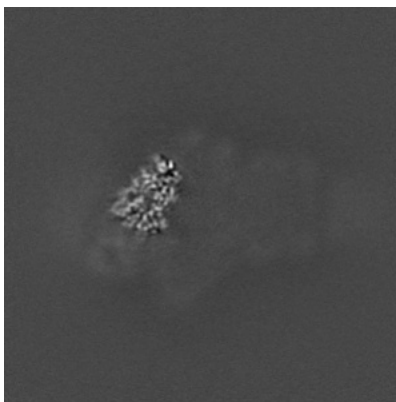


Z Index: 153

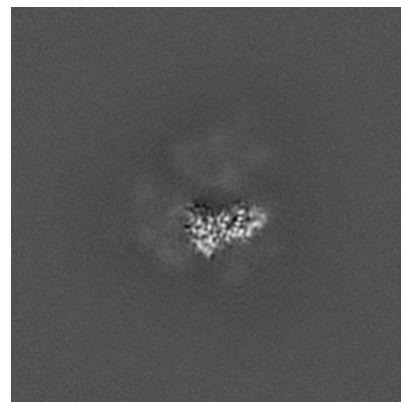
### 6.3.2 Raw map



X Index: 198



Y Index: 180

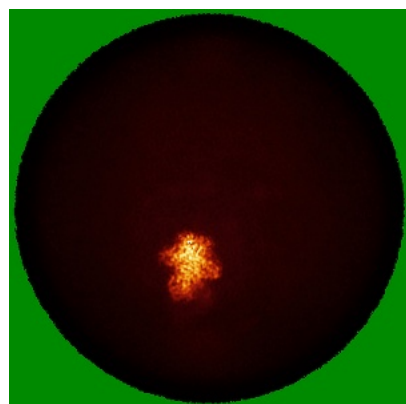


Z Index: 154

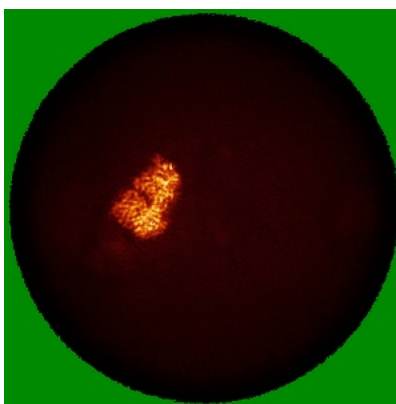
The images above show the largest variance slices of the map in three orthogonal directions.

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

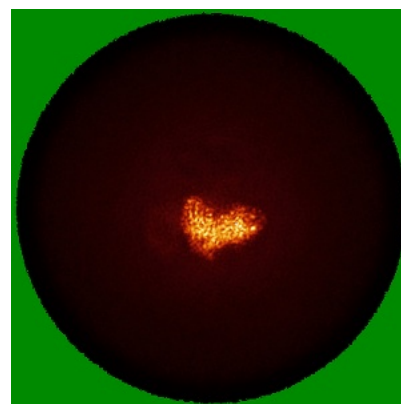
### 6.4.1 Primary map



X

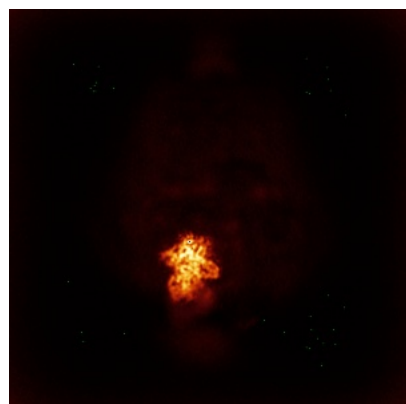


Y

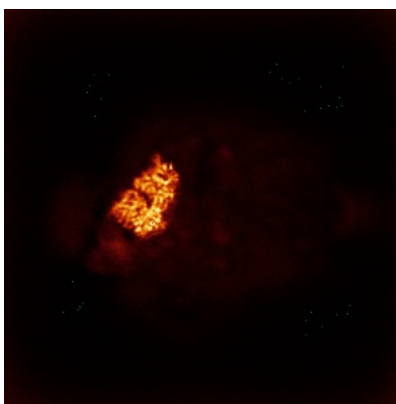


Z

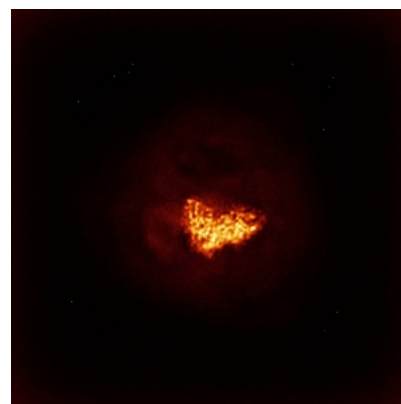
### 6.4.2 Raw map



X



Y

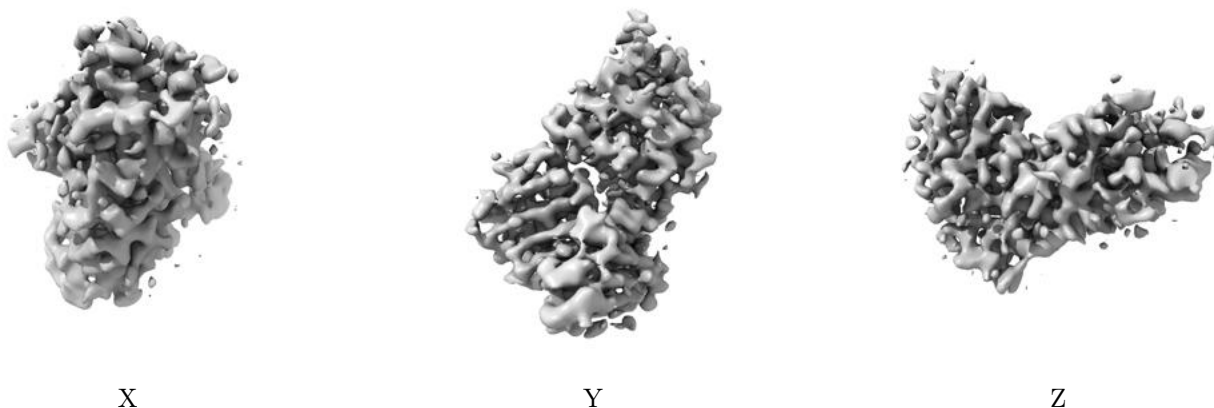


Z

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.

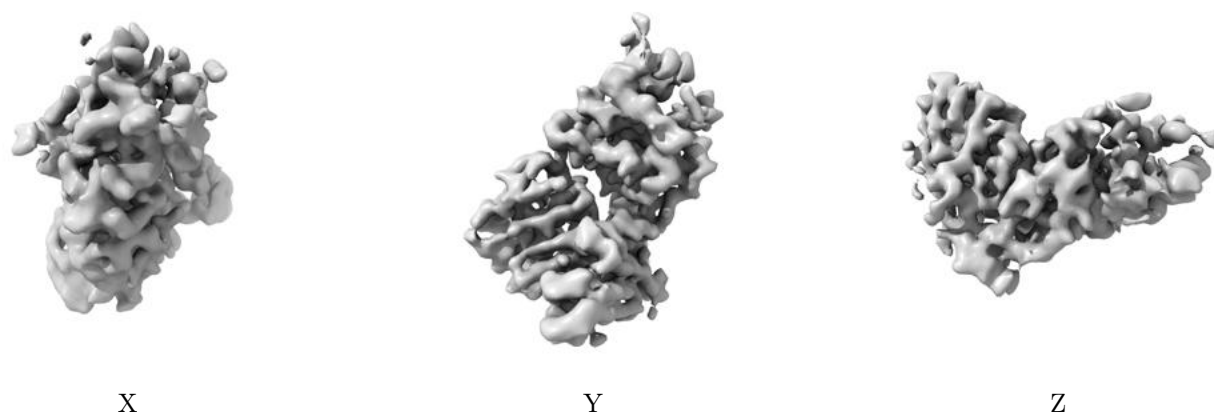
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. 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.

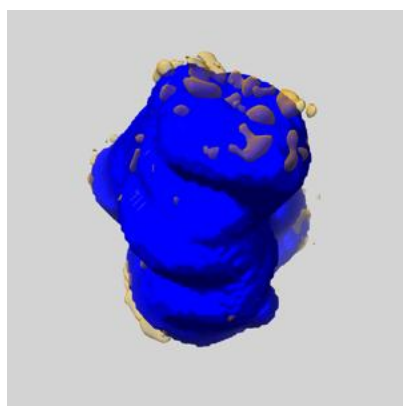
## 6.6 Mask visualisation [i](#)

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

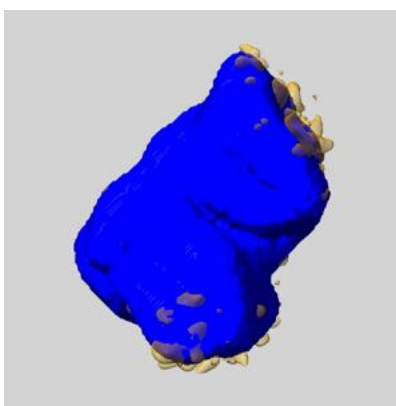
A mask typically either:

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

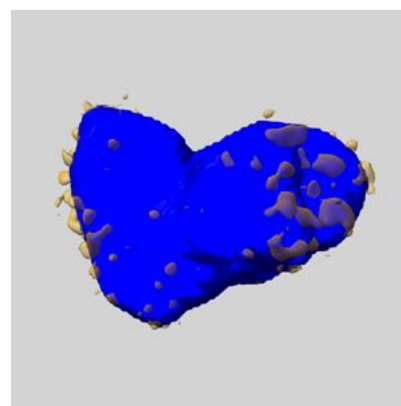
### 6.6.1 emd\_50424\_msk\_1.map [i](#)



X



Y

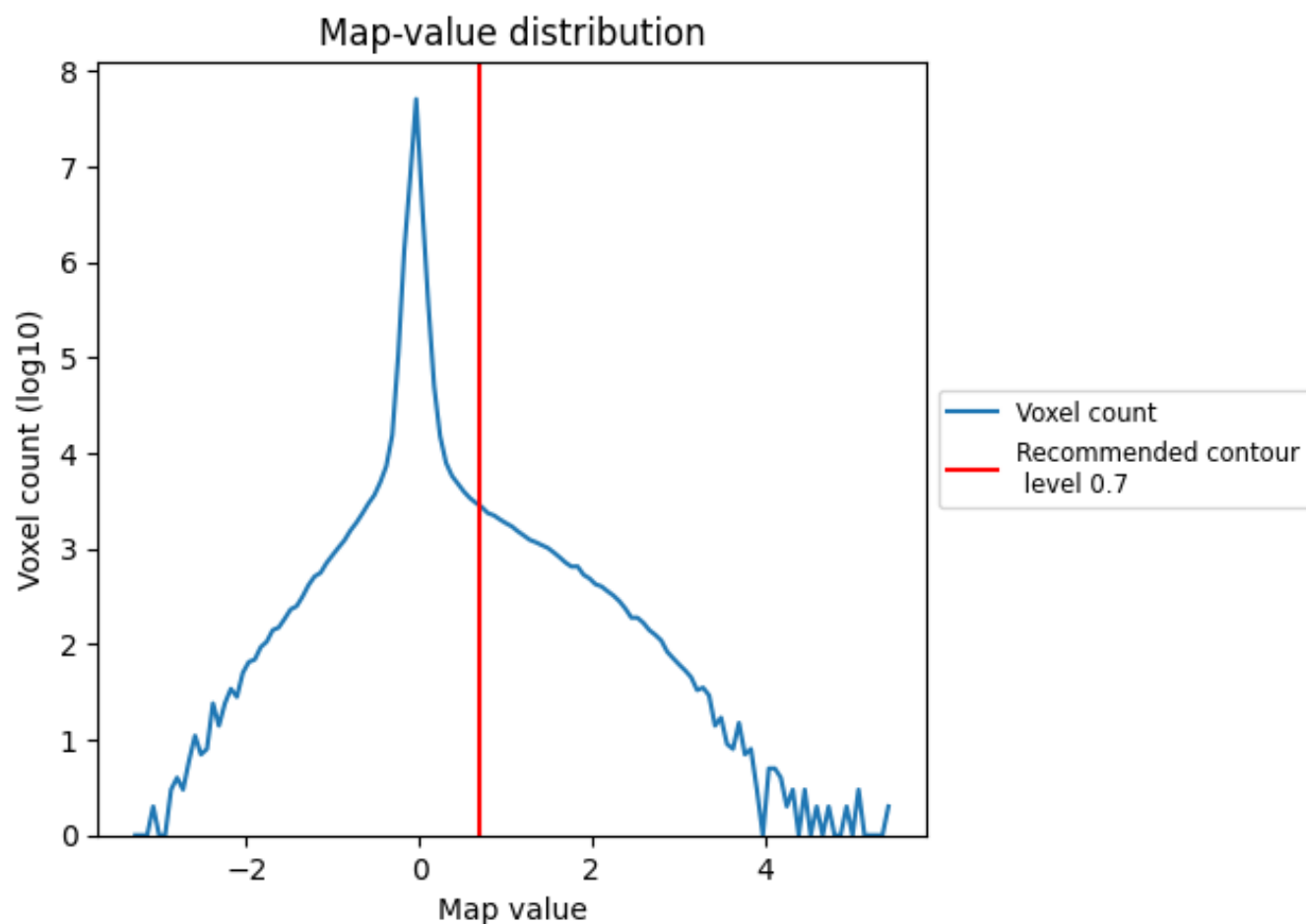


Z

## 7 Map analysis [i](#)

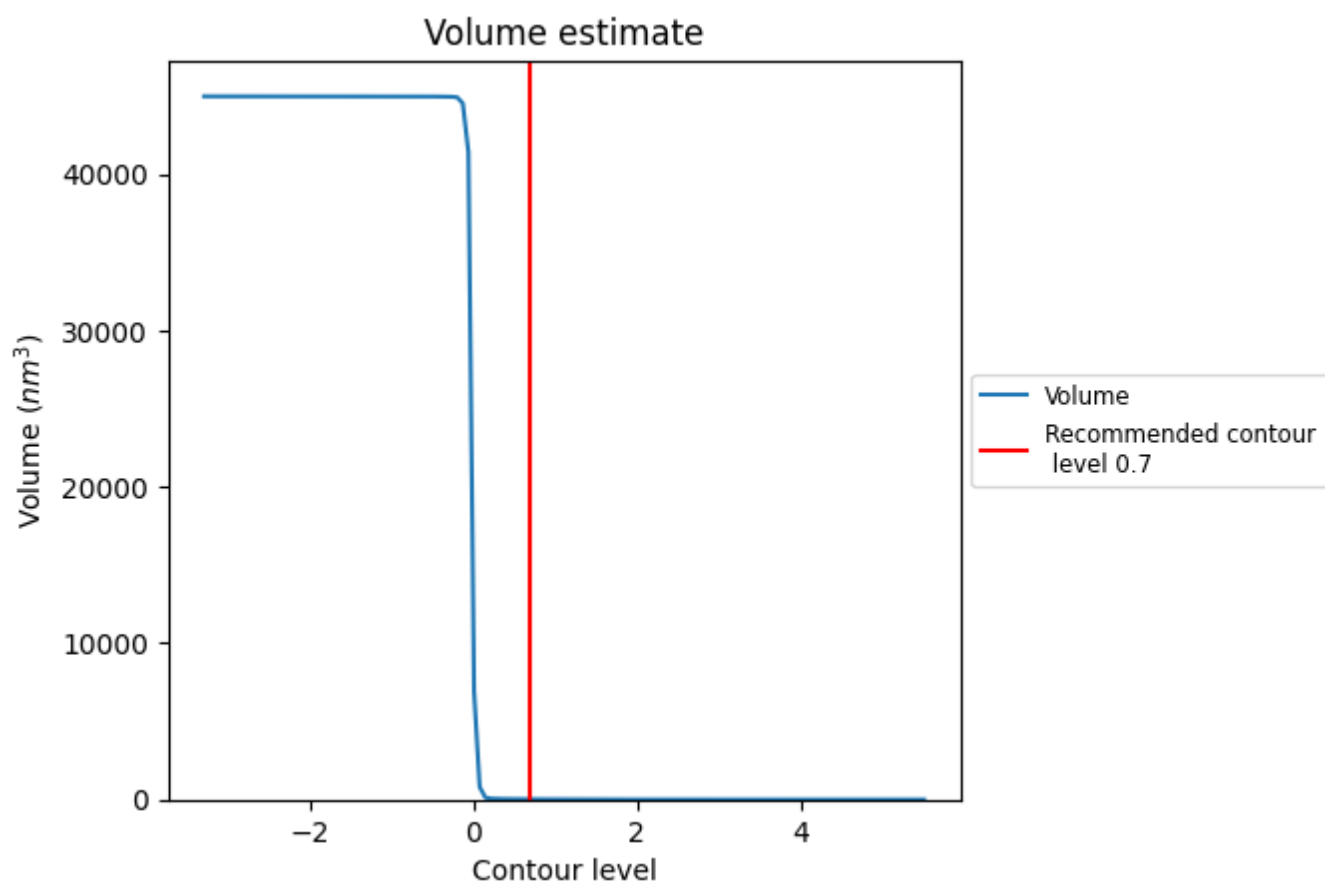
This section contains the results of statistical analysis of the map.

### 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.

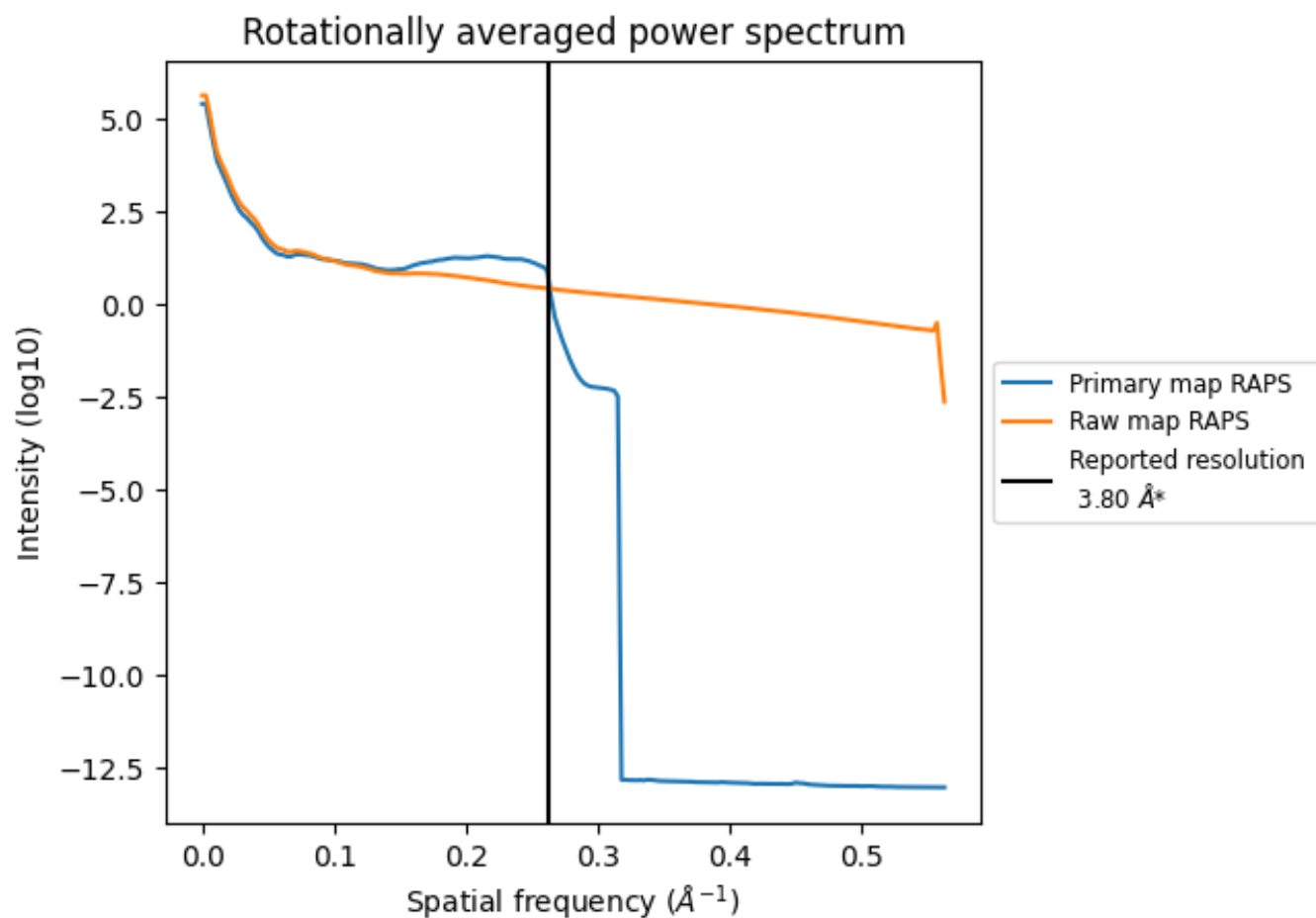
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 21  $\text{nm}^3$ ; this corresponds to an approximate mass of 19 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 ⓘ

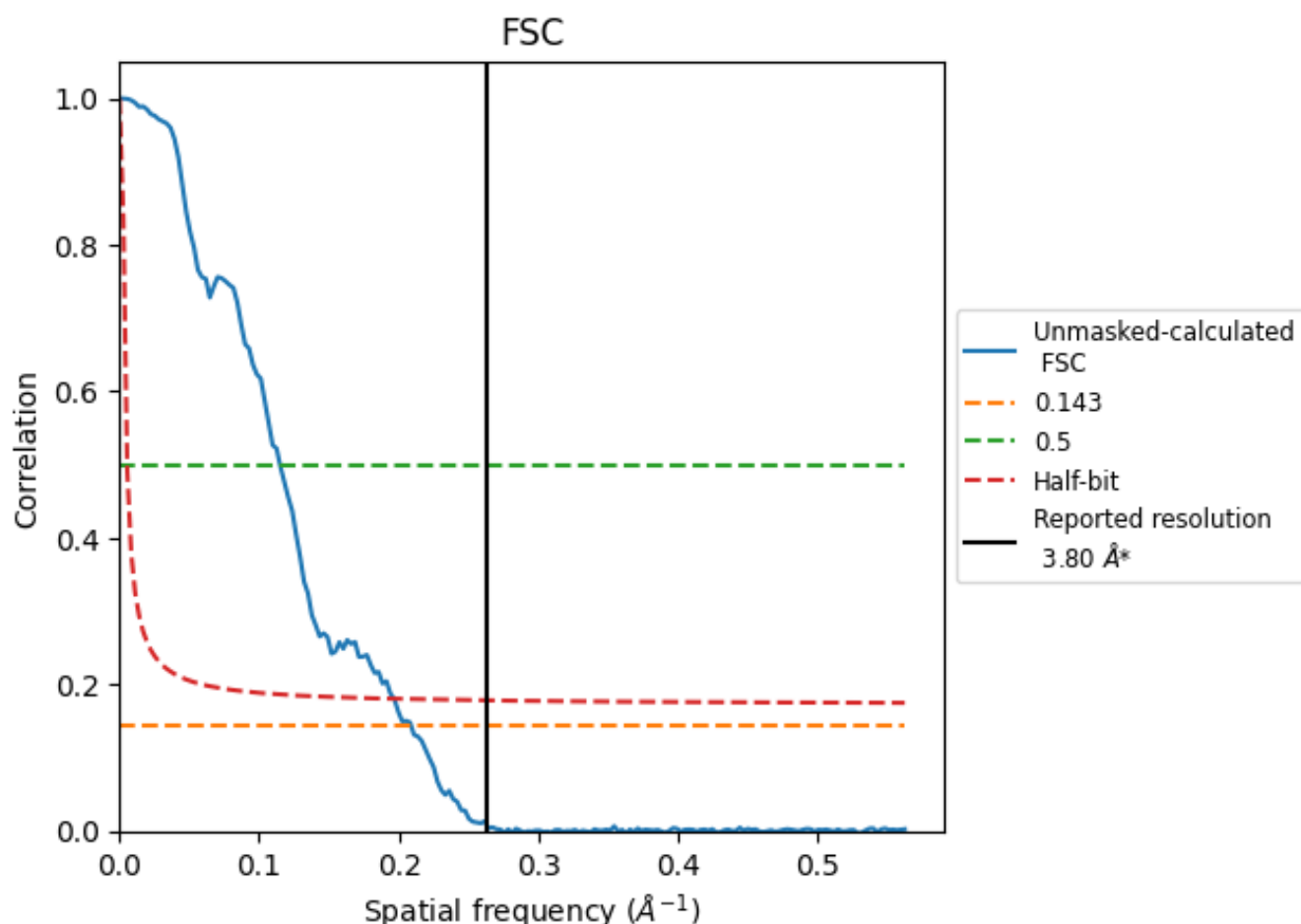


\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

## 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 0.263 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

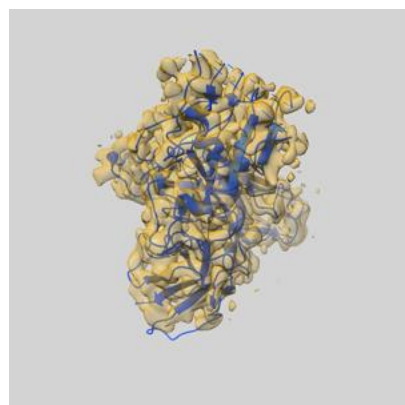
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.79	8.70	5.09

\*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 4.79 differs from the reported value 3.8 by more than 10 %

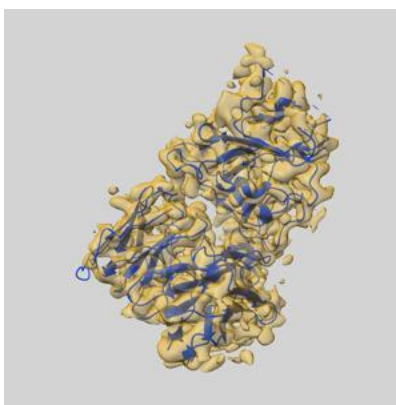
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50424 and PDB model 9FGT. Per-residue inclusion information can be found in section [3](#) on page [8](#).

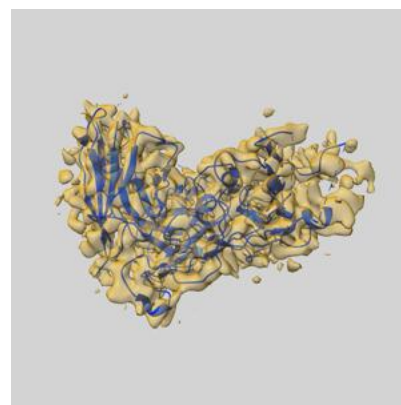
### 9.1 Map-model overlay [i](#)



X



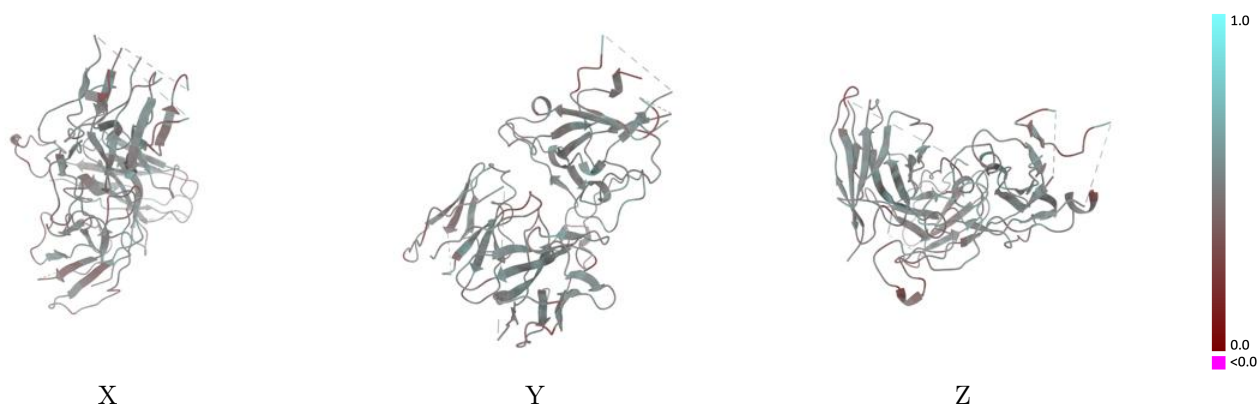
Y



Z

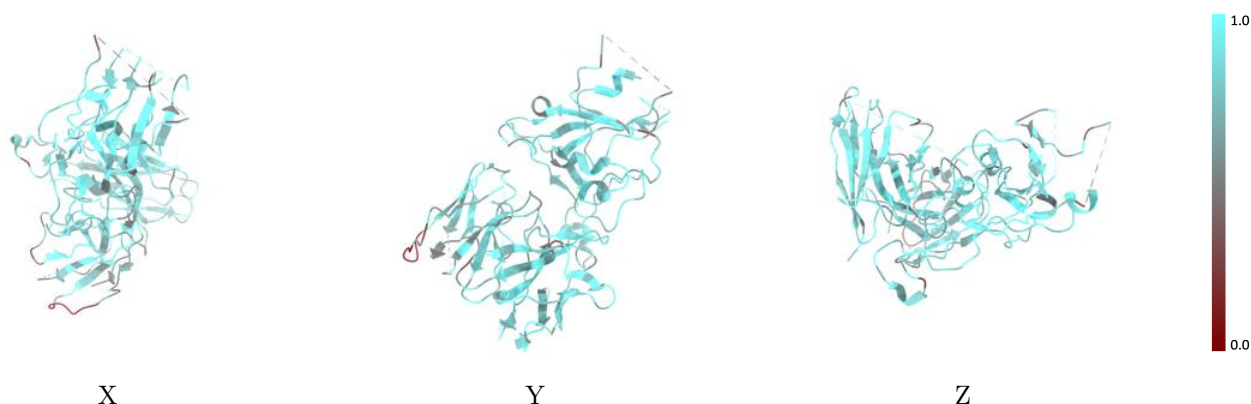
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



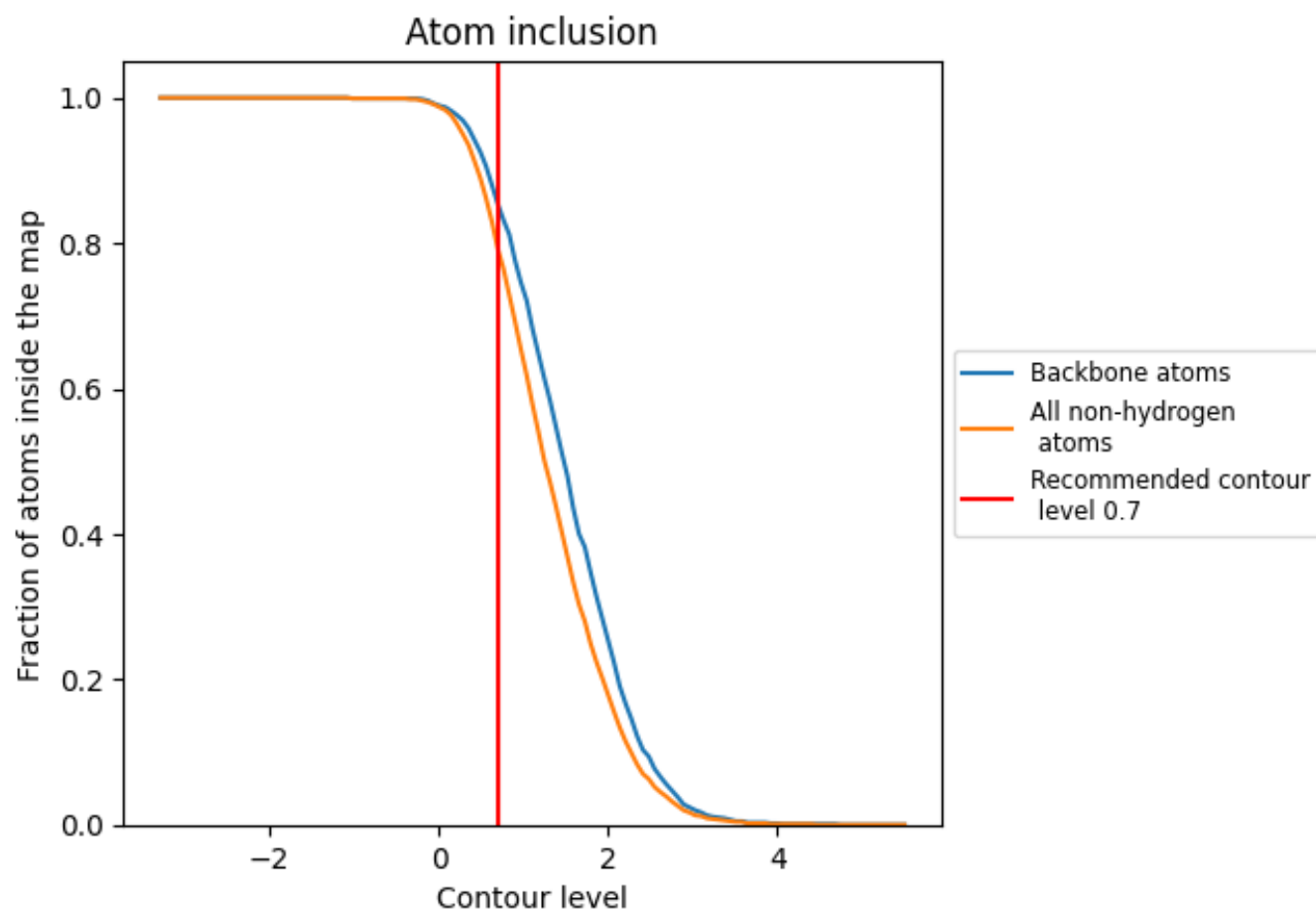
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 79% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7910	<div></div> 0.4790
C	<div></div> 0.8250	<div></div> 0.4810
E	<div></div> 0.7640	<div></div> 0.4780

