



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 12:13 PM UTC

PDB ID : 7FB1 / pdb_00007fb1
EMDB ID : EMD-31512
Title : SARS-CoV-2 spike protein in one-RBD open state
Authors : Zhu, Y.; Tai, L.H.; Sun, F.
Deposited on : 2021-07-08
Resolution : 3.70 Å (reported)

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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:

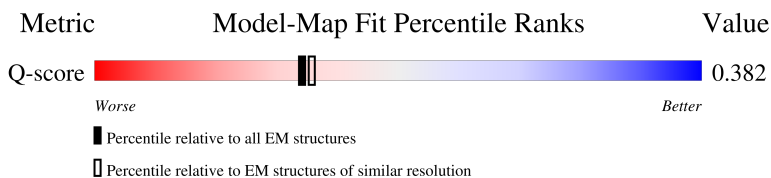
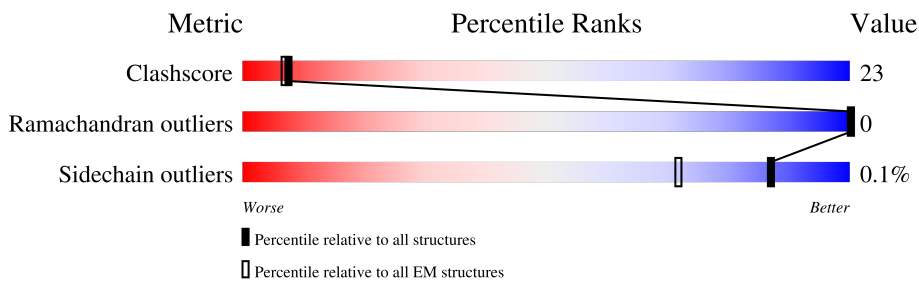
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	1247	<p>6% (poor fit), 48% (0 outliers), 35% (1 outlier), 17% (2+ outliers)</p>
1	B	1247	<p>6% (poor fit), 47% (0 outliers), 36% (1 outlier), 17% (2+ outliers)</p>
1	C	1247	<p>47% (0 outliers), 35% (1 outlier), 17% (2+ outliers)</p>

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 24168 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
			Total	C	N	O	S		
1	A	1029	8039	5133	1338	1530	38	0	0
1	B	1036	8091	5168	1346	1540	37	0	0
1	C	1029	8038	5136	1336	1529	37	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	ALA	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	LEU	-	expression tag	UNP P0DTC2
A	1210	VAL	-	expression tag	UNP P0DTC2
A	1211	PRO	-	expression tag	UNP P0DTC2
A	1212	ARG	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	TYR	-	expression tag	UNP P0DTC2
A	1217	ILE	-	expression tag	UNP P0DTC2
A	1218	PRO	-	expression tag	UNP P0DTC2
A	1219	GLU	-	expression tag	UNP P0DTC2
A	1220	ALA	-	expression tag	UNP P0DTC2
A	1221	PRO	-	expression tag	UNP P0DTC2
A	1222	ARG	-	expression tag	UNP P0DTC2
A	1223	ASP	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLN	-	expression tag	UNP P0DTC2
A	1226	ALA	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1228	VAL	-	expression tag	UNP P0DTC2
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	LYS	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLU	-	expression tag	UNP P0DTC2
A	1234	TRP	-	expression tag	UNP P0DTC2
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	THR	-	expression tag	UNP P0DTC2
A	1240	PHE	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	ALA	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	LEU	-	expression tag	UNP P0DTC2
B	1210	VAL	-	expression tag	UNP P0DTC2
B	1211	PRO	-	expression tag	UNP P0DTC2
B	1212	ARG	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	TYR	-	expression tag	UNP P0DTC2
B	1217	ILE	-	expression tag	UNP P0DTC2
B	1218	PRO	-	expression tag	UNP P0DTC2
B	1219	GLU	-	expression tag	UNP P0DTC2
B	1220	ALA	-	expression tag	UNP P0DTC2
B	1221	PRO	-	expression tag	UNP P0DTC2
B	1222	ARG	-	expression tag	UNP P0DTC2
B	1223	ASP	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1226	ALA	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	VAL	-	expression tag	UNP P0DTC2
B	1229	ARG	-	expression tag	UNP P0DTC2
B	1230	LYS	-	expression tag	UNP P0DTC2
B	1231	ASP	-	expression tag	UNP P0DTC2
B	1232	GLY	-	expression tag	UNP P0DTC2
B	1233	GLU	-	expression tag	UNP P0DTC2
B	1234	TRP	-	expression tag	UNP P0DTC2
B	1235	VAL	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	THR	-	expression tag	UNP P0DTC2
B	1240	PHE	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	ALA	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	LEU	-	expression tag	UNP P0DTC2
C	1210	VAL	-	expression tag	UNP P0DTC2
C	1211	PRO	-	expression tag	UNP P0DTC2
C	1212	ARG	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	TYR	-	expression tag	UNP P0DTC2
C	1217	ILE	-	expression tag	UNP P0DTC2
C	1218	PRO	-	expression tag	UNP P0DTC2
C	1219	GLU	-	expression tag	UNP P0DTC2
C	1220	ALA	-	expression tag	UNP P0DTC2
C	1221	PRO	-	expression tag	UNP P0DTC2
C	1222	ARG	-	expression tag	UNP P0DTC2
C	1223	ASP	-	expression tag	UNP P0DTC2

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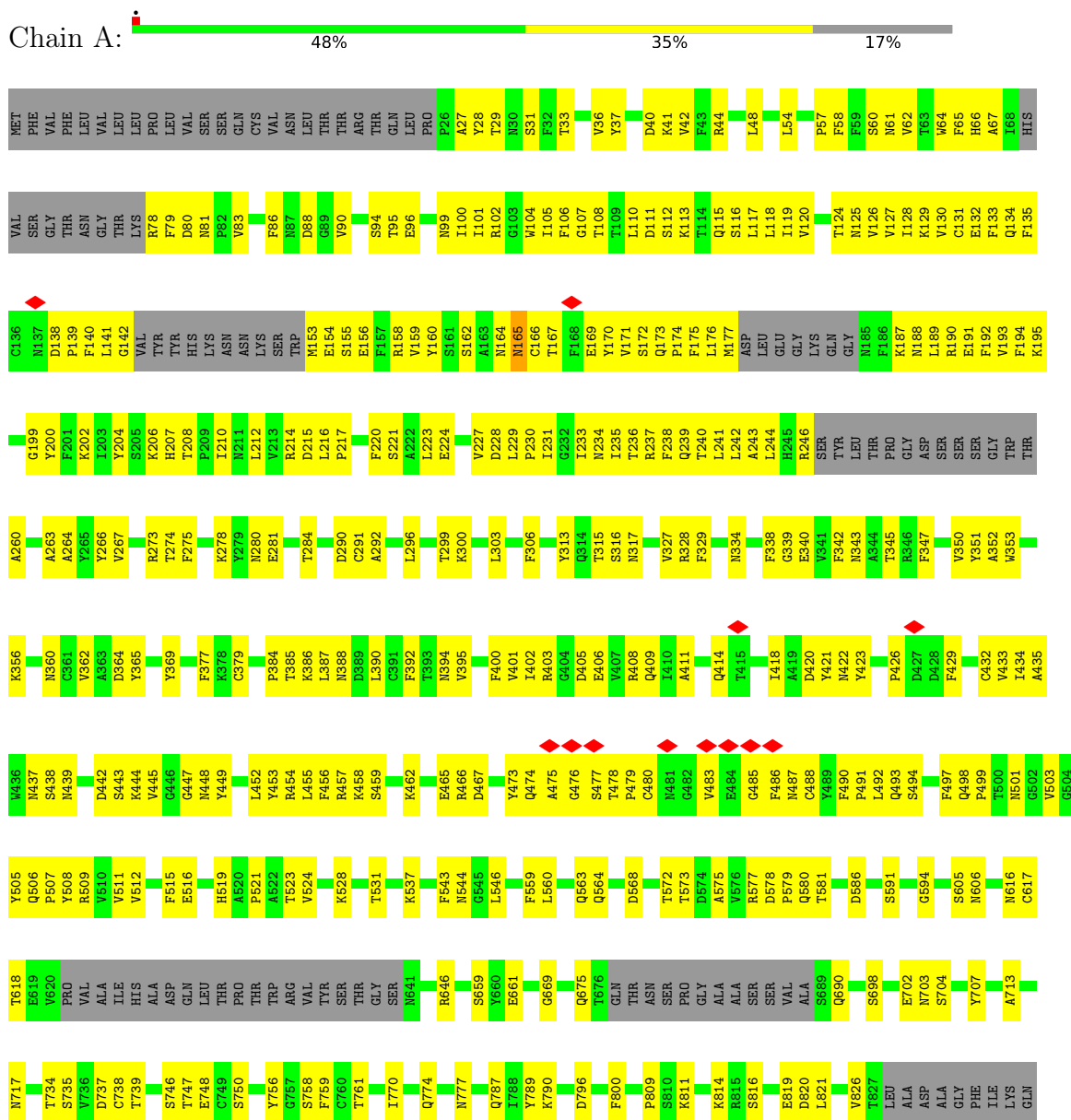
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLN	-	expression tag	UNP P0DTC2
C	1226	ALA	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	VAL	-	expression tag	UNP P0DTC2
C	1229	ARG	-	expression tag	UNP P0DTC2
C	1230	LYS	-	expression tag	UNP P0DTC2
C	1231	ASP	-	expression tag	UNP P0DTC2
C	1232	GLY	-	expression tag	UNP P0DTC2
C	1233	GLU	-	expression tag	UNP P0DTC2
C	1234	TRP	-	expression tag	UNP P0DTC2
C	1235	VAL	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	THR	-	expression tag	UNP P0DTC2
C	1240	PHE	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2

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



ILE	V1137	S1003	A879	L806	SER	S591
ASP	Y1138	Q1010	T883	P809	SER	F592
LEU	L1141	R1014	S884	K810	VAL	V597
GLN	Q1142	K1028	L894	P812	ALA	S605
LEU	P1143	R905	Q901	S813	ALA	N606
GLY	E1144	F906	R907	K814	ALA	V615
LYS	L1145	N907	G908	S815	ALA	N616
TYR	D1146	I909	I910	F908	ALA	C617
GLU	SER	F1042	G911	S704	ALA	V620
GLN	PHE	H1048	T912	I714	PRO	PRO
LEU	LYS	L1049	Y917	E725	VAL	VAL
VAL	LYS	Q1054	L922	V826	ALA	ALA
PRO	ASN	S1055	I923	T827	ALA	ALA
ARG	HIS	A1056	A924	LEU	GLN	GLN
GLY	THR	F1057	N925	ALA	LEU	LEU
GLY	SER	H1058	Q926	PHE	THR	THR
TYR	PRO	V1065	F927	ILE	PRO	PRO
ILE	ASP	E1072	N928	LYS	THR	THR
PRO	VAL	T1077	D936	TYR	ARG	ARG
PRO	ASN	A1078	S937	TYR	VAL	VAL
GLU	HIS	T1083	L938	GLY	VAL	VAL
ALA	THR	D1084	S939	ASP	TYR	TYR
ALA	SER	G1085	S940	CYS	SER	SER
VAL	PRO	F1089	T941	LEU	THR	THR
VAL	ASP	P1090	A942	GLY	GLY	GLY
LEU	VAL	E1092	L945	ILE	SER	SER
LEU	VAL	G1093	D950	ALA	GLY	GLY
SER	ASN	V1094	N953	ALA	SER	SER
THR	ILE	S1097	Q965	ALA	THR	THR
THR	ILE	W1102	L966	ALA	TRP	TRP
PHE	GLN	Q1106	N969	ALA	ARG	ARG
LEU	LYS	R1107	A972	ARG	VAL	VAL
HIS	GLU	D1118	S974	ARG	LEU	LEU
HIS	ILE	V976	S975	THR	HIS	HIS
HIS	ASP	N1125	V976	D867	HIS	HIS
HIS	ARG	C1126	D979	E868	HIS	HIS
HIS	ILE	I980	I980	M869	HIS	HIS
HIS	ASN	V1129	R983	I870	HIS	HIS
HIS	GLU	M1135	L984	T866	HIS	HIS
HIS	VAL	T1136	R1000	T866	HIS	HIS
HIS	ALA			D867	HIS	HIS
HIS	LYS			E868	HIS	HIS
HIS	ASN			M869	HIS	HIS
HIS	ASN			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	ASN			D867	HIS	HIS
HIS	GLU			E868	HIS	HIS
HIS	ASN			M869	HIS	HIS
HIS	ASN			I870	HIS	HIS
HIS	ASN			T866	HIS	HIS
HIS	GLU			D867	HIS	HIS
HIS	SER			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
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HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
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HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
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HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
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HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
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HIS	LEU			M869	HIS	HIS
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HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS	LEU			M869	HIS	HIS
HIS	LEU			I870	HIS	HIS
HIS	LEU			T866	HIS	HIS
HIS	LEU			D867	HIS	HIS
HIS	LEU			E868	HIS	HIS
HIS						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50585	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 ($e^-/\text{\AA}^2$)	3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.334	Depositor
Minimum map value	-0.912	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	348.16, 348.16, 348.16	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/8220	0.49	0/11181
1	B	0.33	0/8274	0.53	3/11258 (0.0%)
1	C	0.33	0/8219	0.49	0/11183
All	All	0.33	0/24713	0.50	3/33622 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	VAL	CA-C-N	13.63	138.94	120.67
1	B	83	VAL	C-N-CA	13.63	138.94	120.67
1	B	79	PHE	N-CA-C	-5.32	105.49	112.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	329	PHE	Peptide

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	8039	0	7854	388	0
1	B	8091	0	7907	378	0
1	C	8038	0	7859	364	0
All	All	24168	0	23620	1097	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 23.

The worst 5 of 1097 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:C:825:LYS:HE2	1:C:942:ALA:CB	1.57	1.33
1:C:825:LYS:CE	1:C:942:ALA:HB2	1.70	1.20
1:C:825:LYS:CE	1:C:942:ALA:CB	2.26	1.11
1:C:945:LEU:HD23	1:C:945:LEU:H	1.21	1.04
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.40	1.04

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	1013/1247 (81%)	869 (86%)	144 (14%)	0	100	100
1	B	1020/1247 (82%)	886 (87%)	134 (13%)	0	100	100
1	C	1012/1247 (81%)	878 (87%)	134 (13%)	0	100	100
All	All	3045/3741 (81%)	2633 (86%)	412 (14%)	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	A	898/1085 (83%)	897 (100%)	1 (0%)	88	88
1	B	905/1085 (83%)	905 (100%)	0	100	100
1	C	899/1085 (83%)	898 (100%)	1 (0%)	88	88
All	All	2702/3255 (83%)	2700 (100%)	2 (0%)	87	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	C	945	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	388	ASN
1	C	949	GLN
1	C	519	HIS
1	C	717	ASN
1	C	1036	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](#)

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.

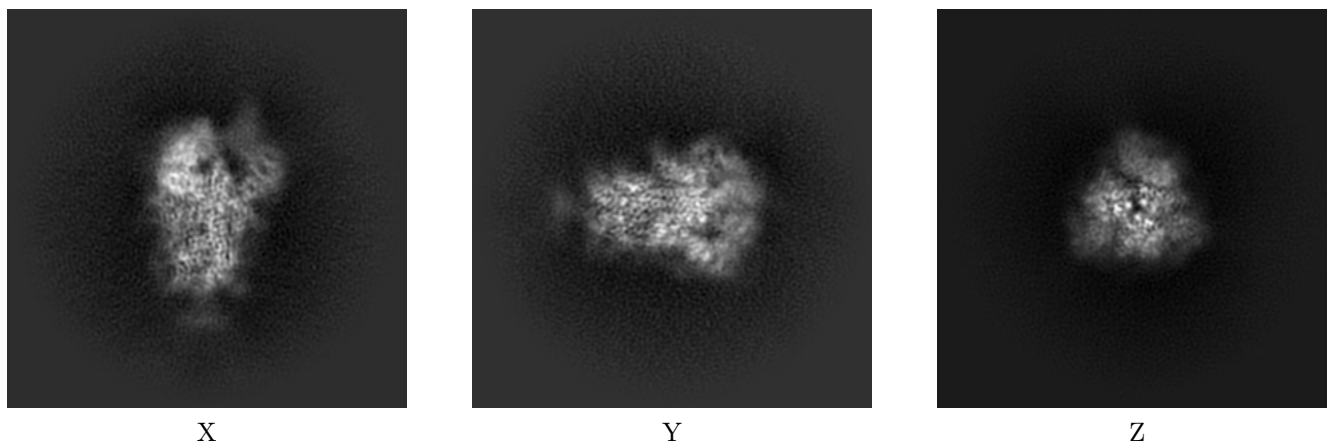
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31512. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

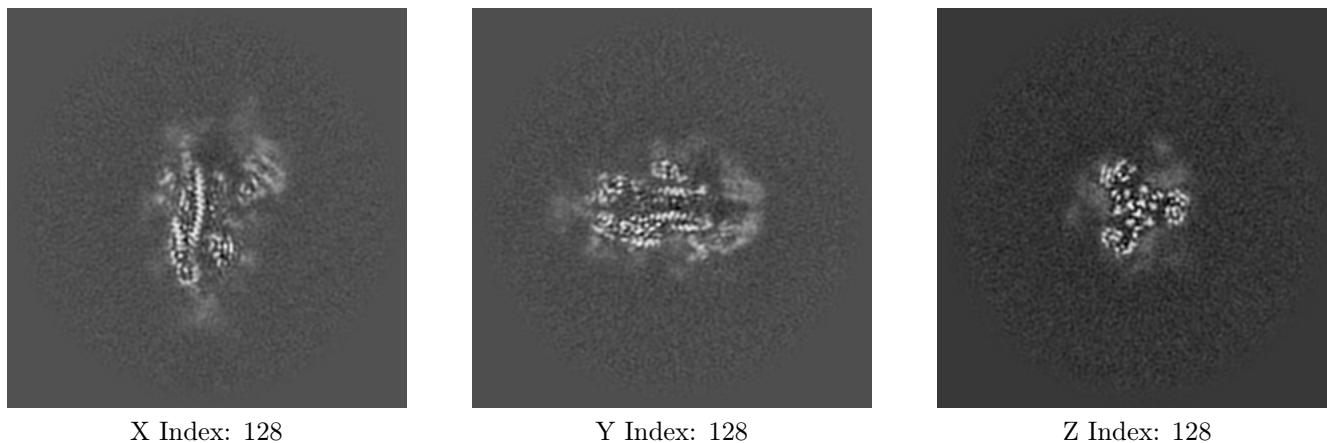
6.1.1 Primary map



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

6.2 Central slices [i](#)

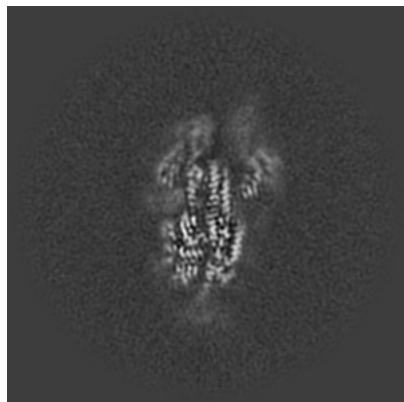
6.2.1 Primary map



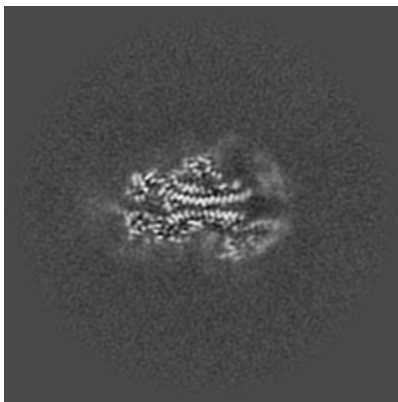
The images above show central slices of the map in three orthogonal directions.

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

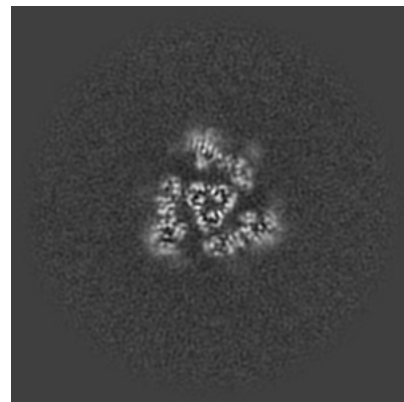
6.3.1 Primary map



X Index: 133



Y Index: 131

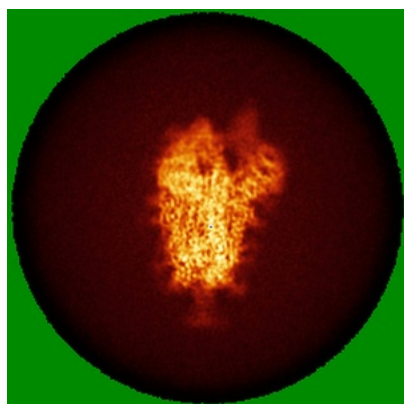


Z Index: 147

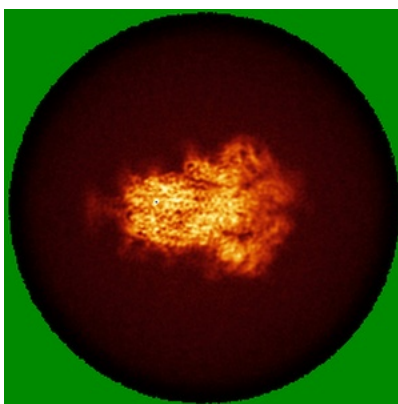
The images above show the largest variance slices of the map in three orthogonal directions.

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

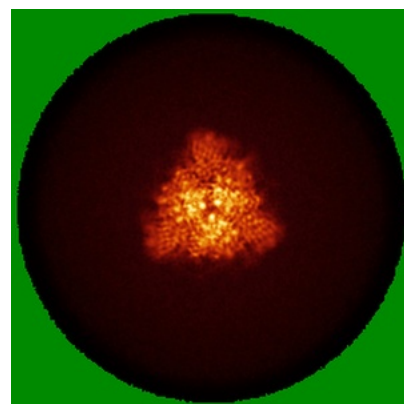
6.4.1 Primary map



X



Y

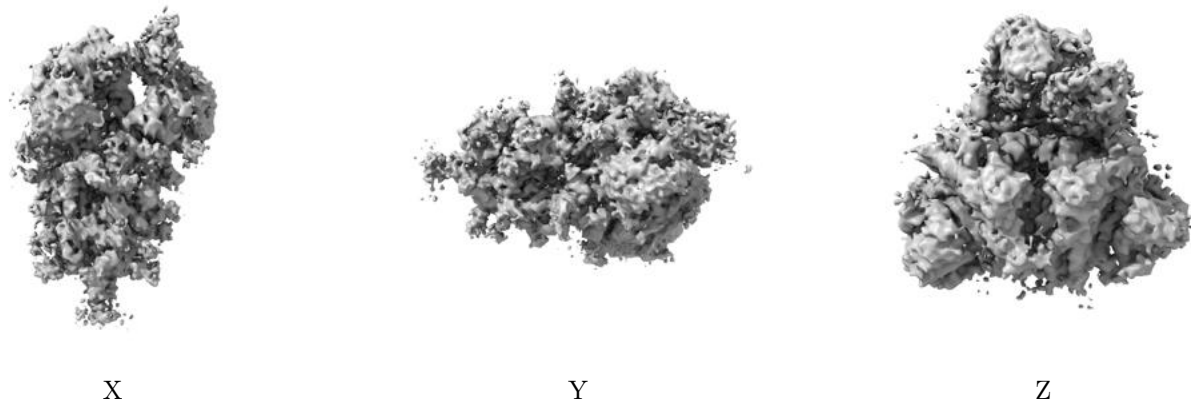


Z

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 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

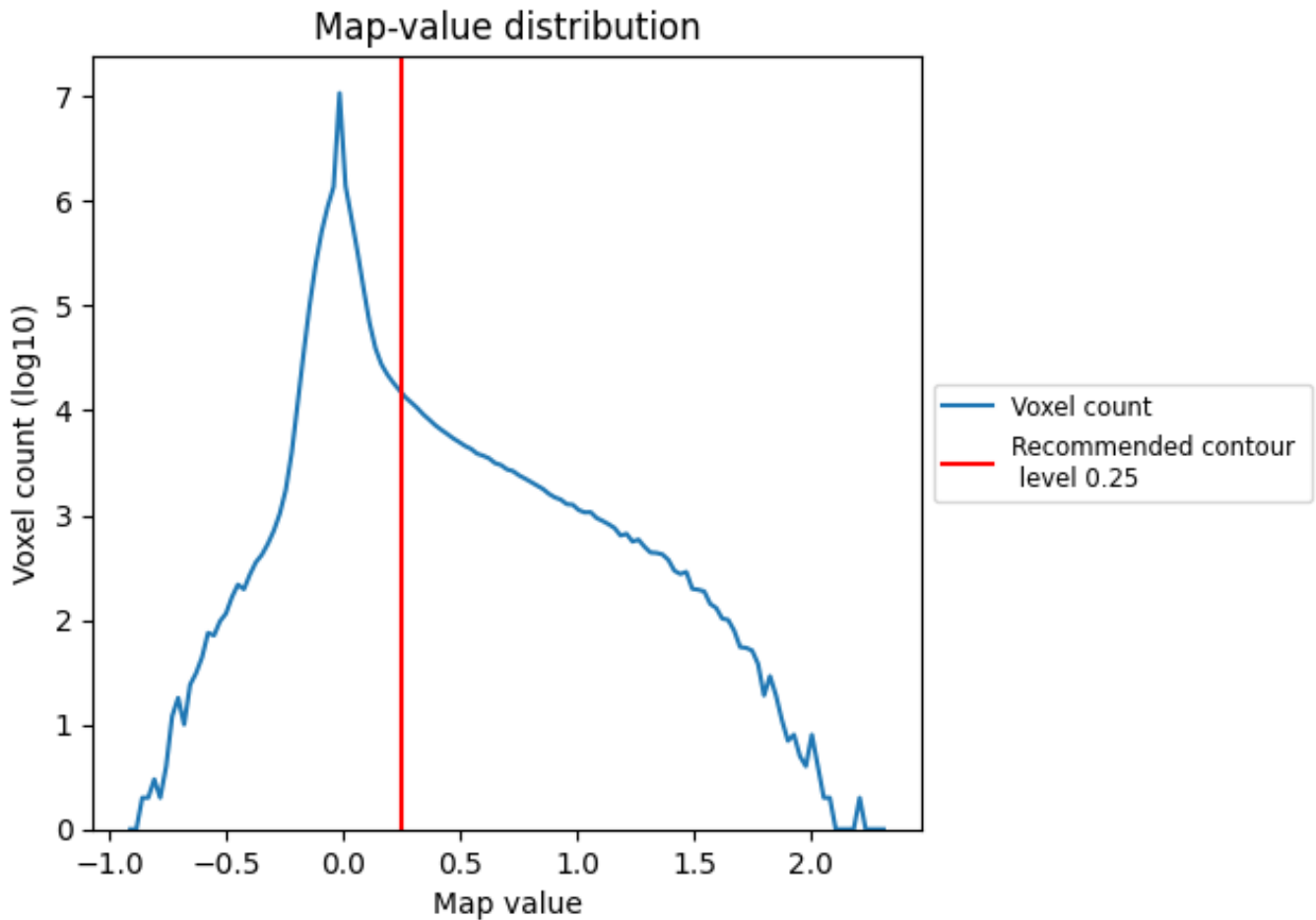
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

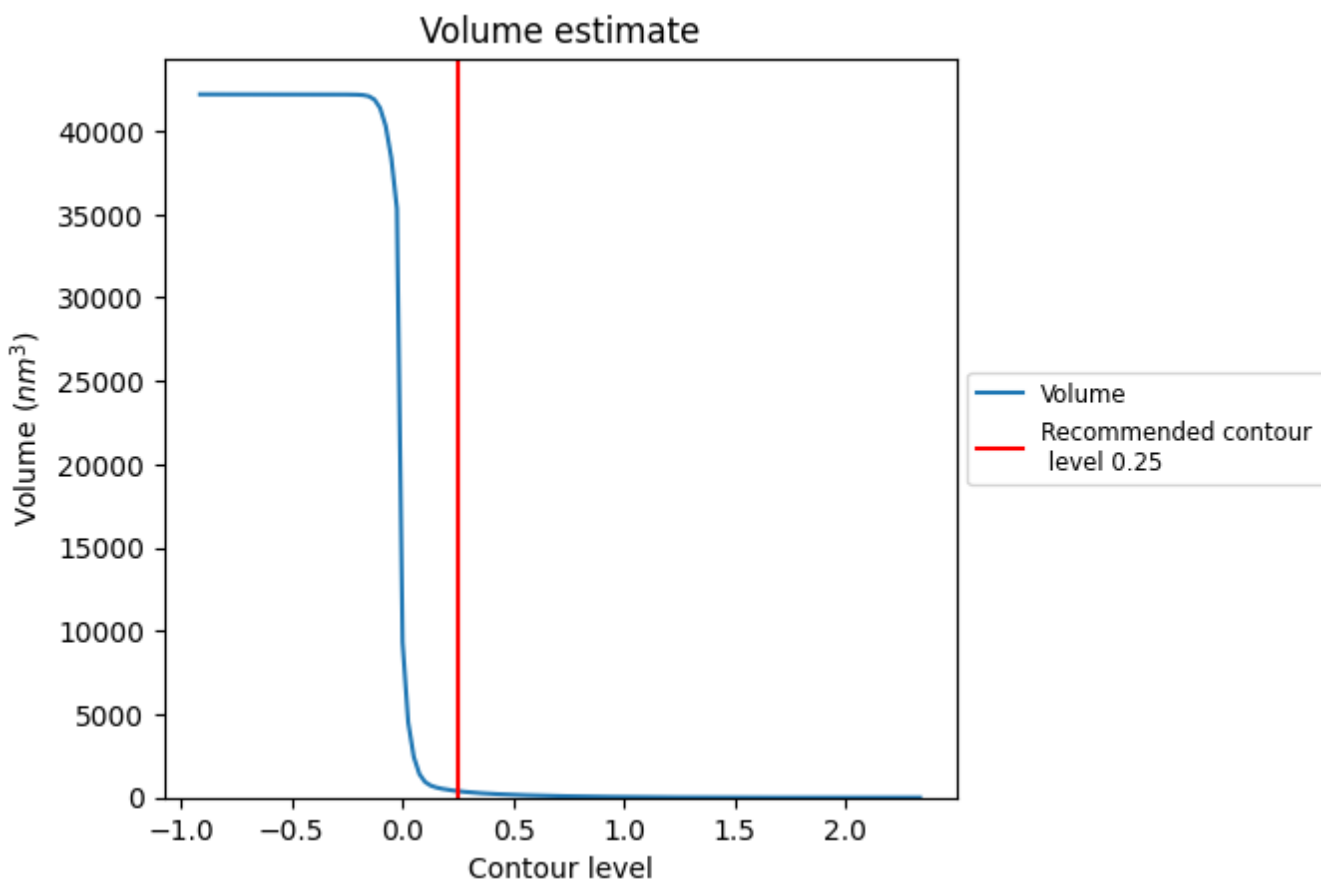
This section contains the results of statistical analysis of the map.

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.

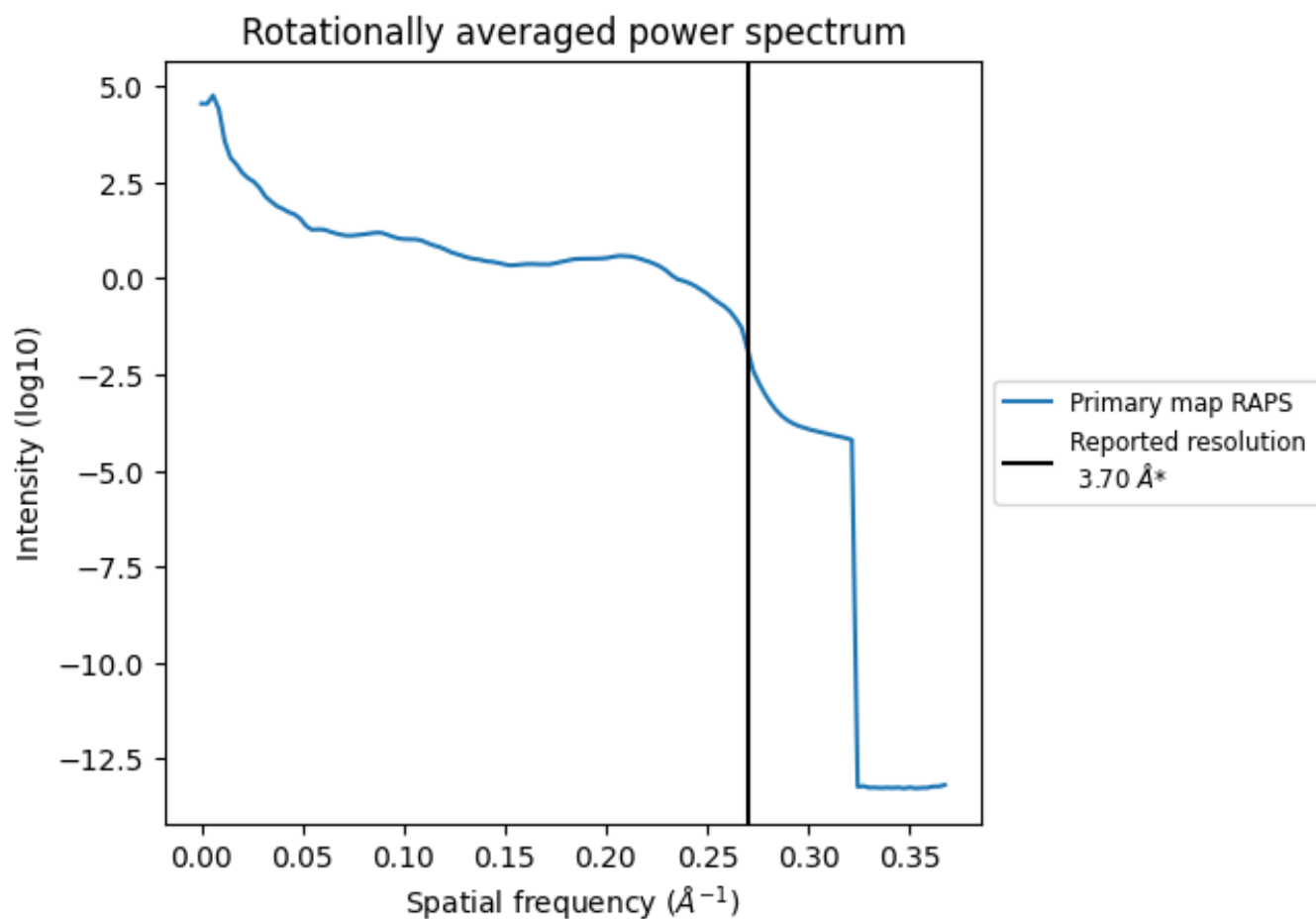
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 387 nm³; this corresponds to an approximate mass of 350 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 [i](#)

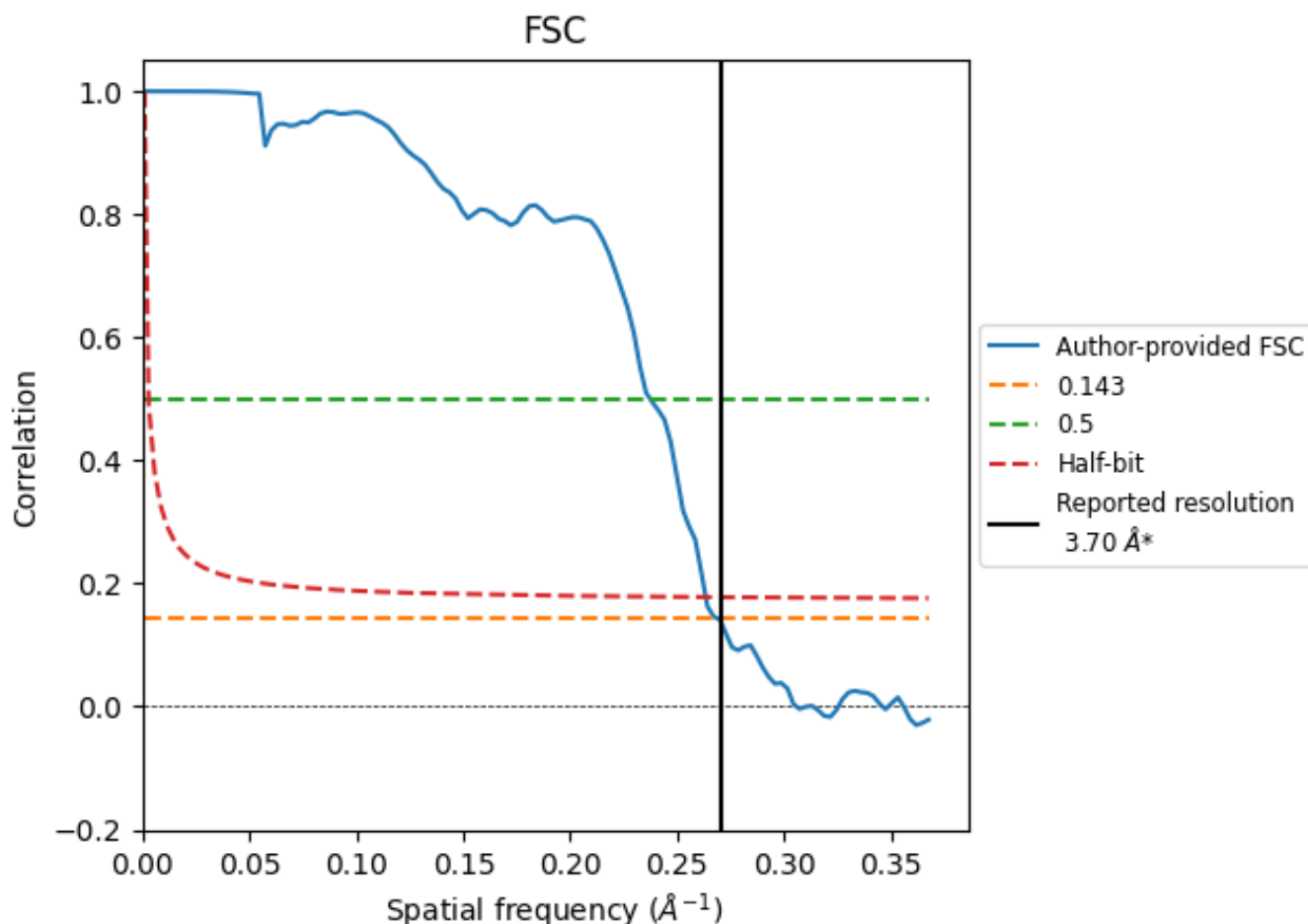


*Reported resolution corresponds to spatial frequency of 0.270\AA^{-1}

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

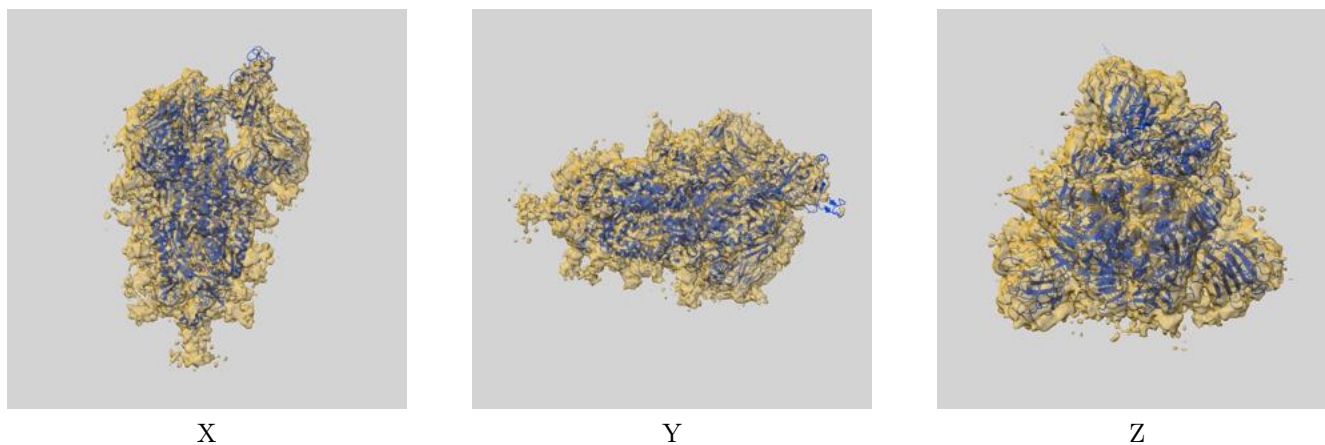
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.72	4.21	3.80
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

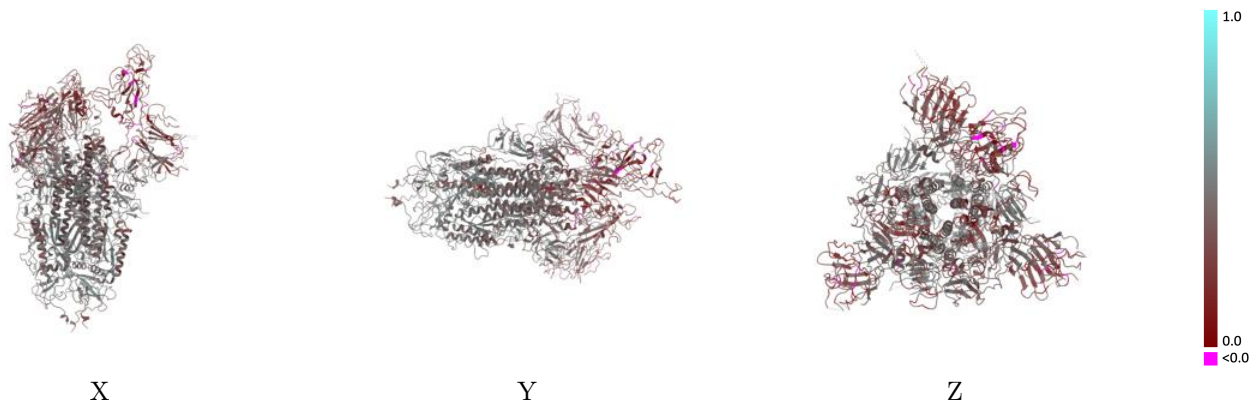
This section contains information regarding the fit between EMDB map EMD-31512 and PDB model 7FB1. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.25 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](#)

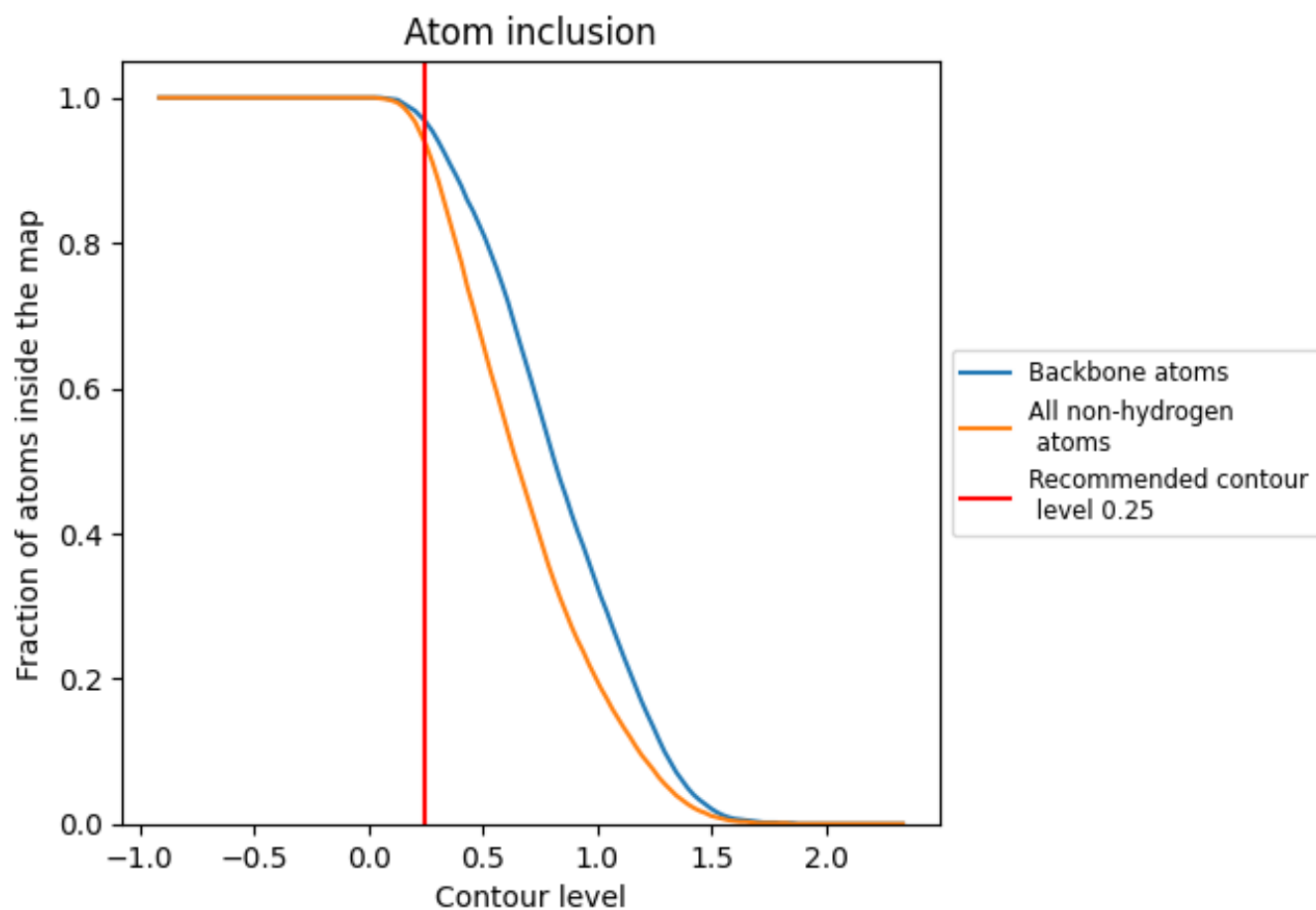


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.









9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9360	 0.3820
A	 0.9540	 0.3860
B	 0.8920	 0.3750
C	 0.9630	 0.3860

