



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 08:12 PM EDT

PDB ID : 8TM1
EMDB ID : EMD-41374
Title : Antibody N3-1 bound to RBDs in the up and down conformations
Authors : Hsieh, C.-L.; McLellan, J.S.
Deposited on : 2023-07-27
Resolution : 2.79 Å(reported)

This is a Full wwPDB EM Validation 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

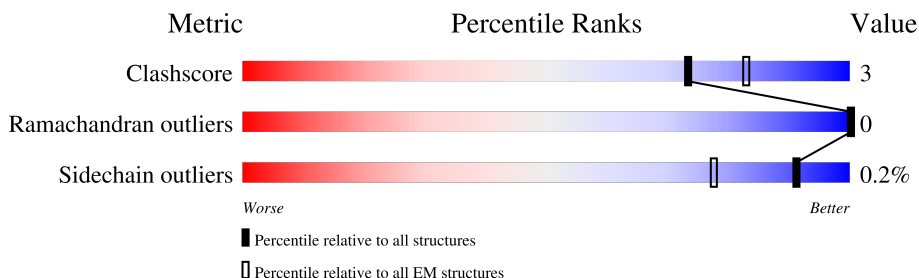
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1288	
1	B	1288	
2	H	128	
3	L	108	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4536 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	175	Total	C	N	O	S	0	0
			1407	908	233	261	5		
1	B	159	Total	C	N	O	S	0	0
			1282	825	215	238	4		

There are 178 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	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	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	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 N3-1 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	127	Total	C	N	O	S	0	0
			1015	650	171	191	3		

- Molecule 3 is a protein called N3-1 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	108	Total	C	N	O	S	0	0
			832	525	135	169	3		

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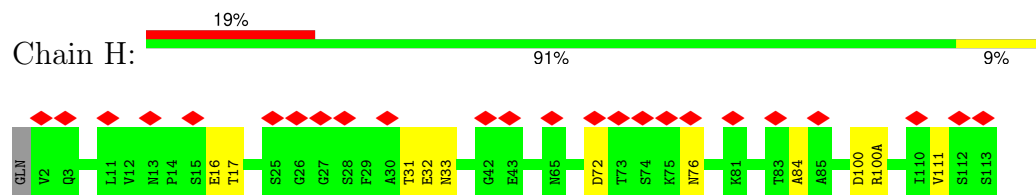
- Molecule 1: Spike glycoprotein



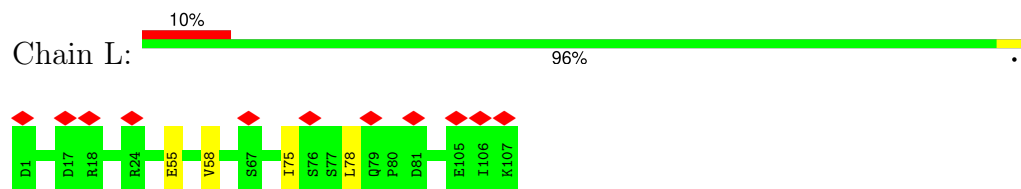
ALA	ILE	ALA	GLY	LEU	F374	CYS	LEU	GLY	ASN	MET
PRO	PRO	THR	HIS	VAL	C379	THR	LEU	GLN	VAL	PHE
THR	THR	VAL	ASN	ASN	Y380	LYS	ALA	GLN	THR	THR
PHE	ASN	VAL	LYS	CYS	GLY	SER	HIS	ASN	PHE	LEU
THR	THR	THR	VAL	VAL	VAL	THR	SER	PHE	HIS	VAL
ILE	THR	GLY	ASN	THR	THR	VAL	TYR	ASN	ILE	LEU
VAL	CYS	THR	ASN	LYS	LYS	THR	THR	ARG	VAL	VAL
THR	THR	THR	ASN	LEU	ILE	GLY	PRO	GLU	CYS	VAL
GLY	THR	THR	ASN	ASN	THR	TYR	GLY	PHE	GLY	THR
ILE	ASN	GLY	THR	GLY	N394	PHE	THR	ASP	THR	LEU
LEU	GLN	THR	LEU	LEU	V395	ARG	THR	THR	ARG	LEU
PRO	ALA	VAL	GLY	PHE	K417	VAL	ALA	GLY	THR	THR
ALA	VAL	VAL	ALA	THR	THR	THR	ALA	ILE	ASN	ASN
VAL	VAL	VAL	ASN	GLY	D427	GLY	ALA	TYR	LYS	PRO
SER	ILE	VAL	VAL	GLY	D428	SER	TYR	SER	PRO	PRO
MET	CYS	CYS	THR	VAL	C432	ILE	VAL	LYS	ASN	ALA
THR	ALA	THR	ALA	LEU	V445	PHE	GLY	THR	ASN	THR
LYS	SER	GLN	THR	THR	G446	ARG	LEU	THR	GLY	VAL
THR	THR	VAL	VAL	VAL	G447	PRO	LEU	ILE	VAL	VAL
SER	THR	ASN	ALA	GLY	N448	THR	ARG	VAL	THR	THR
VAL	THR	VAL	ALA	GLY	Y449	ASN	PHE	ARG	GLU	ARG
ASP	CYS	GLN	CYS	ASP	N450	CYS	LEU	ASP	SER	GLY
THR	THR	ALA	LEU	ASP	R457	PRO	LEU	LEU	THR	VAL
CYS	SER	GLN	THR	ILE	D467	F338	LEU	PRO	LYS	TYR
ASN	ASN	THR	ALA	ALA	THR	G339	LEU	GLN	ASN	THR
LEU	LEU	ILE	THR	THR	THR	E340	THR	PHE	ILE	THR
LEU	THR	THR	THR	THR	Q498	THR	GLY	ASN	SER	LYS
LEU	ALA	ARG	ASP	ASP	N501	R346	ASN	ALA	ARG	VAL
TYR	THR	VAL	VAL	VAL	F515	R357	GLY	LEU	GLY	PHE
GLY	SER	ARG	THR	THR	GLU	I368	ILE	PRO	ASN	THR
SER	SER	THR	THR	GLY	LEU	S359	THR	LEU	CYS	SER
PHE	THR	GLY	SER	GLN	LEU	ASN	ALA	ASP	THR	LEU
CYS	THR	ALA	ASN	THR	HIS	CYS	VAL	VAL	GLY	THR
GLN	VAL	GLY	VAL	GLY	ALA	ALA	ASP	CYS	ILE	THR
ARG	VAL	THR	THR	LEU	ALA	ASP	LEU	ILE	GLN	LYS
ALA	ALA	ARG	ASP	VAL	VAL	S366	THR	ASN	PRO	THR
LEU	THR	ALA	ILE	ILE	GLY	V367	PRO	ILE	PHE	PHE
THR	THR	GLY	THR	THR	CYS	I368	LEU	THR	GLN	THR
GLY	ASN	CYS	THR	CYS	GLY	Y369	THR	ARG	LEU	LEU
ILE	ASN	PRO	PRO	PRO	LYS	N370	GLU	PHE	LEU	PHE
ALA	THR	LYS	LYS	THR	THR	THR	THR	GLN	ILE	THR

[illegible]

- Molecule 2: N3-1 Fab heavy chain



- Molecule 3: N3-1 Fab light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	266553	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	12.571	Depositor
Minimum map value	-6.927	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.167	Depositor
Recommended contour level	2.66	Depositor
Map size (\AA)	475.2, 475.2, 475.2	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/1447	0.52	0/1964
1	B	0.26	0/1317	0.53	0/1784
2	H	0.26	0/1048	0.56	0/1430
3	L	0.24	0/853	0.54	0/1159
All	All	0.25	0/4665	0.54	0/6337

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	408	ARG	Sidechain
1	B	457	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1407	0	1332	12	0
1	B	1282	0	1208	7	0
2	H	1015	0	950	6	0
3	L	832	0	796	3	0
All	All	4536	0	4286	27	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.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:NH1	1:A:358:ILE:O	2.31	0.63
2:H:84:ALA:HA	2:H:111:VAL:HG21	1.81	0.61
2:H:31:THR:HG22	2:H:33:ASN:H	1.66	0.60
1:A:406:GLU:OE1	1:A:409:GLN:NE2	2.35	0.59
2:H:16:GLU:HG3	2:H:17:THR:H	1.71	0.55
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.44	0.53
1:A:473:TYR:HD1	1:A:491:PRO:HD3	1.73	0.52
1:B:457:ARG:NH1	1:B:467:ASP:OD2	2.43	0.52
1:A:457:ARG:NH1	1:A:459:SER:O	2.38	0.47
1:A:490:PHE:HE2	1:A:492:LEU:HB2	1.79	0.47
1:A:408:ARG:NH1	3:L:55:GLU:OE1	2.49	0.46
1:B:448:ASN:OD1	1:B:450:ASN:ND2	2.45	0.45
2:H:100:ASP:OD1	2:H:100(A):ARG:N	2.49	0.45
1:A:357:ARG:NH2	1:A:393:THR:O	2.48	0.45
1:A:349:SER:OG	1:A:452:LEU:O	2.36	0.43
2:H:16:GLU:HG3	2:H:17:THR:N	2.33	0.43
1:A:490:PHE:CD1	1:A:491:PRO:HD2	2.55	0.42
2:H:72:ASP:O	2:H:76:ASN:N	2.52	0.42
3:L:55:GLU:O	3:L:58:VAL:HG22	2.19	0.42
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.56	0.41
1:A:419:ALA:HA	1:A:423:TYR:O	2.20	0.41
3:L:75:ILE:HG21	3:L:78:LEU:HD23	2.03	0.41
1:B:379:CYS:HA	1:B:432:CYS:HA	2.02	0.40
1:B:498:GLN:HB2	1:B:501:ASN:OD1	2.22	0.40
1:B:368:LEU:HA	1:B:374:PHE:HE2	1.86	0.40
1:B:417:LYS:HA	1:B:417:LYS:HD3	1.95	0.40
1:B:395:VAL:HG12	1:B:515:PHE:HD1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	171/1288 (13%)	167 (98%)	4 (2%)	0	100	100
1	B	153/1288 (12%)	150 (98%)	3 (2%)	0	100	100
2	H	125/128 (98%)	119 (95%)	6 (5%)	0	100	100
3	L	106/108 (98%)	100 (94%)	6 (6%)	0	100	100
All	All	555/2812 (20%)	536 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	151/1116 (14%)	151 (100%)	0	100	100
1	B	137/1116 (12%)	137 (100%)	0	100	100
2	H	110/111 (99%)	109 (99%)	1 (1%)	75	92
3	L	93/94 (99%)	93 (100%)	0	100	100
All	All	491/2437 (20%)	490 (100%)	1 (0%)	91	97

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

Mol	Chain	Res	Type
2	H	32	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	460	ASN
1	A	501	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

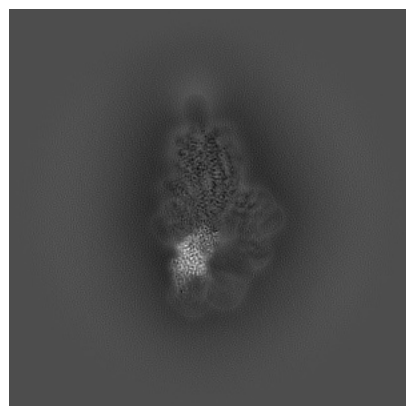
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41374. These allow visual inspection of the internal detail of the map and identification of artifacts.

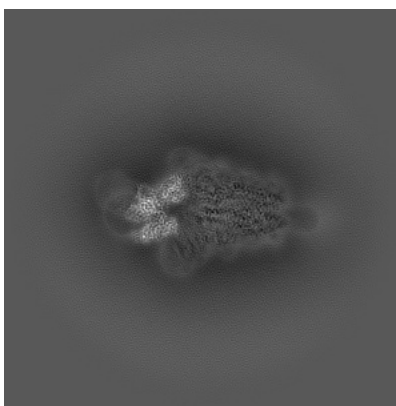
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

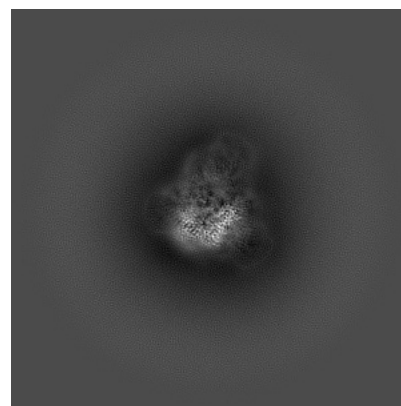
6.1.1 Primary map



X

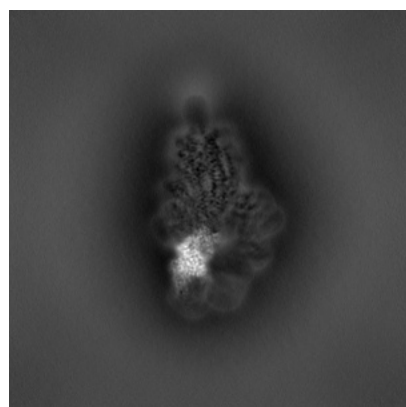


Y

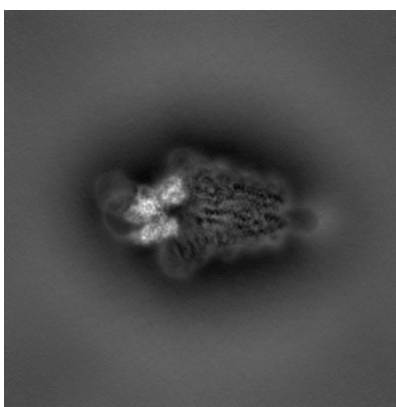


Z

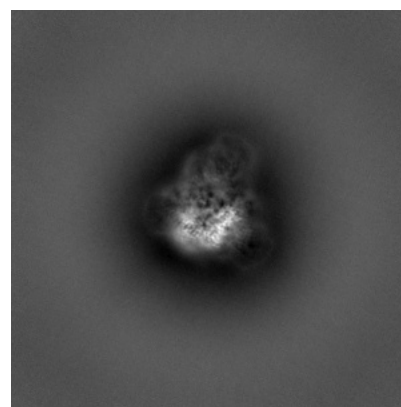
6.1.2 Raw map



X



Y

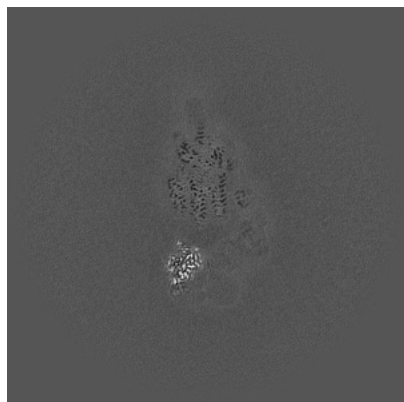


Z

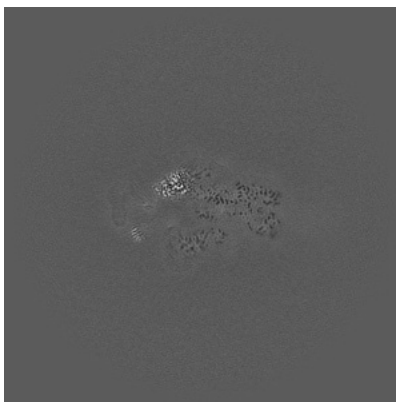
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

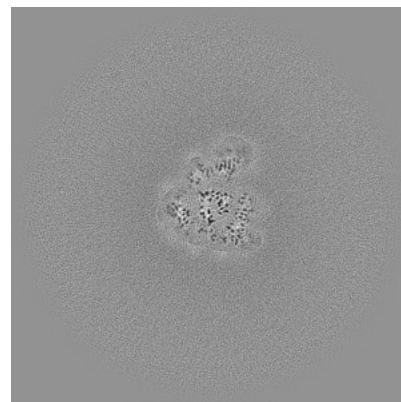
6.2.1 Primary map



X Index: 216

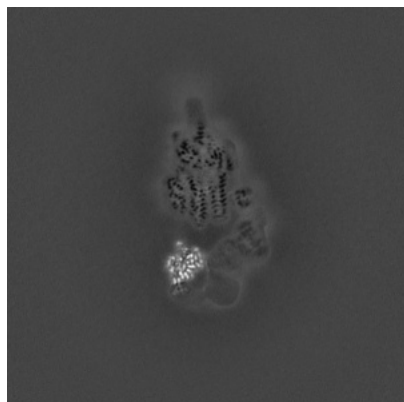


Y Index: 216

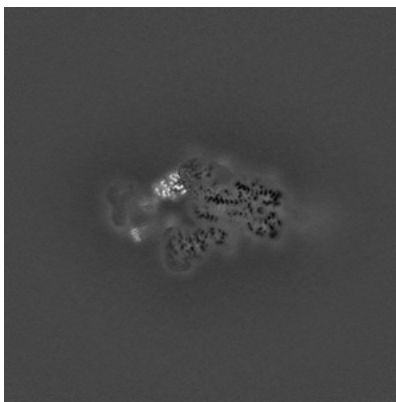


Z Index: 216

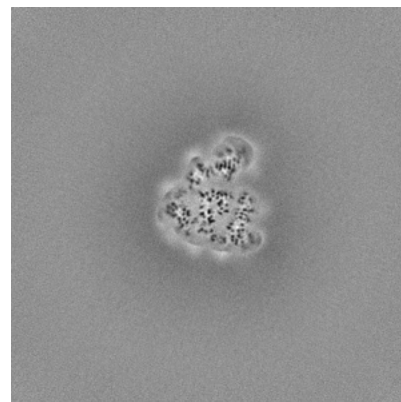
6.2.2 Raw map



X Index: 216



Y Index: 216

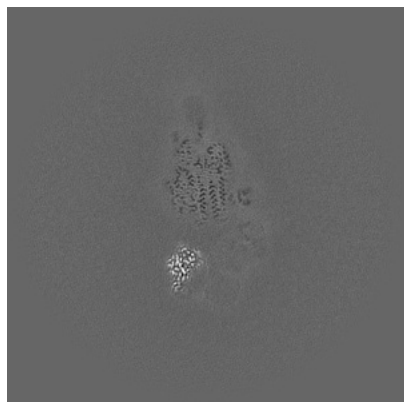


Z Index: 216

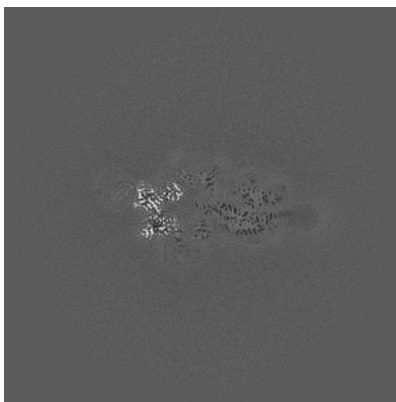
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

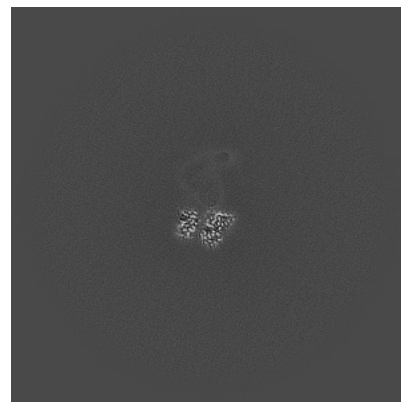
6.3.1 Primary map



X Index: 214

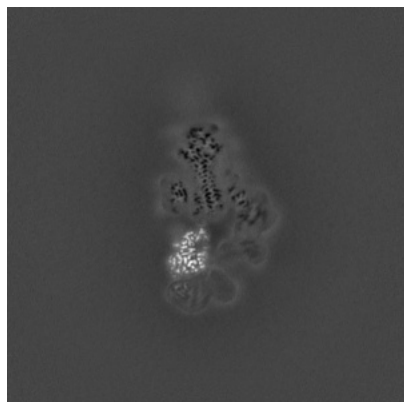


Y Index: 199

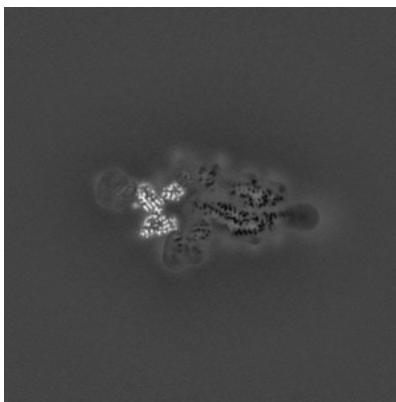


Z Index: 155

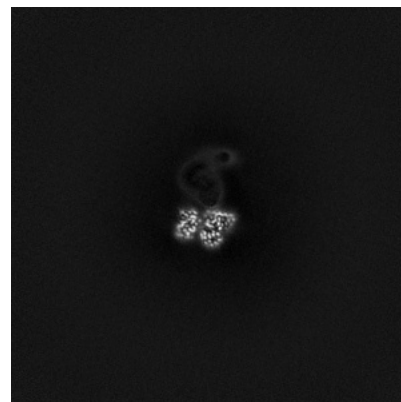
6.3.2 Raw map



X Index: 224



Y Index: 200

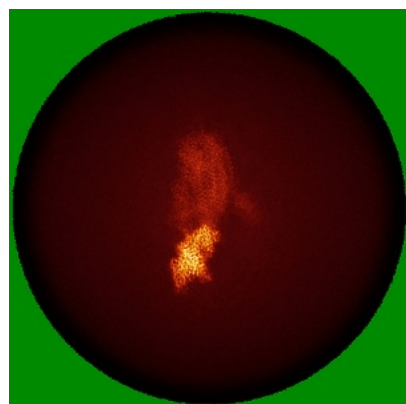


Z Index: 155

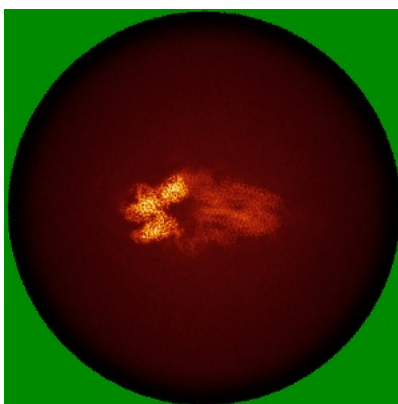
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

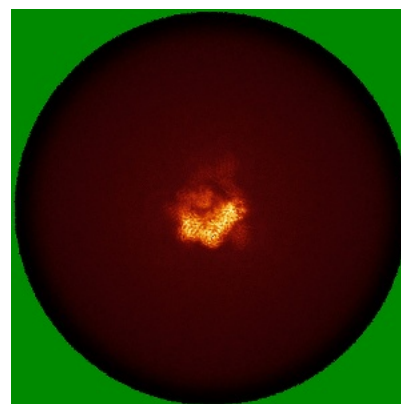
6.4.1 Primary map



X

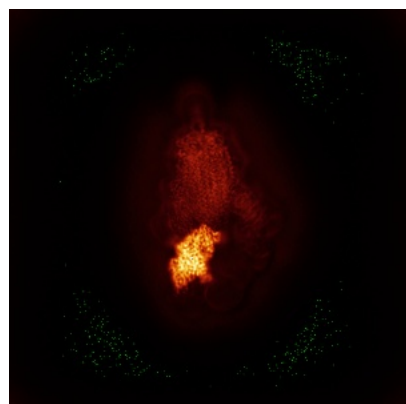


Y

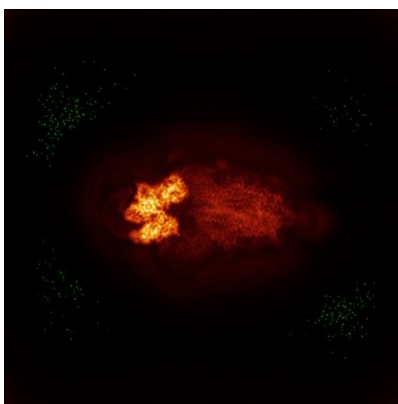


Z

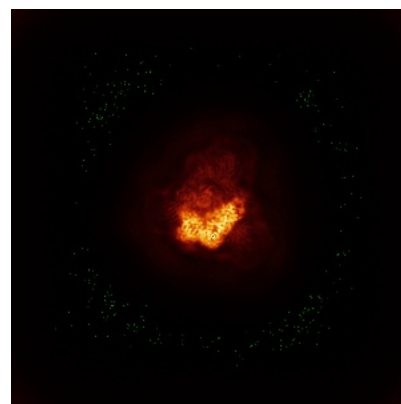
6.4.2 Raw map



X



Y

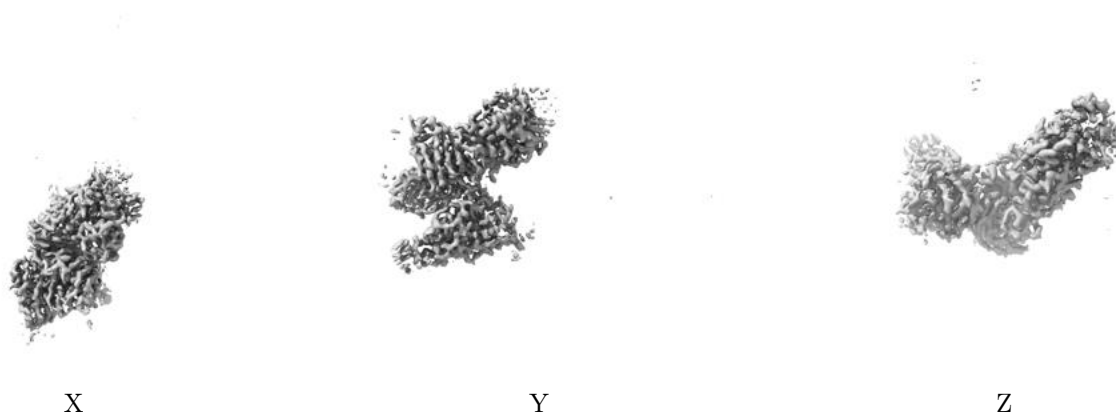


Z

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.

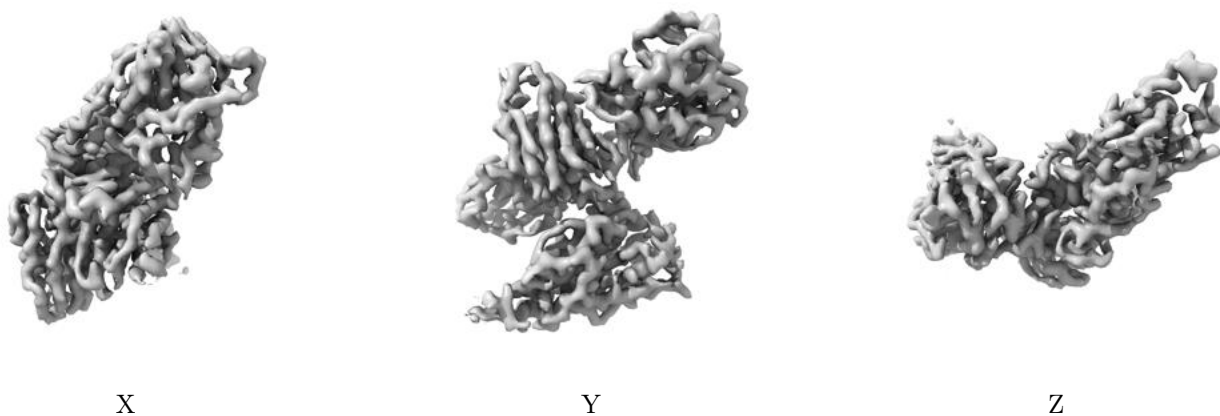
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.66. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

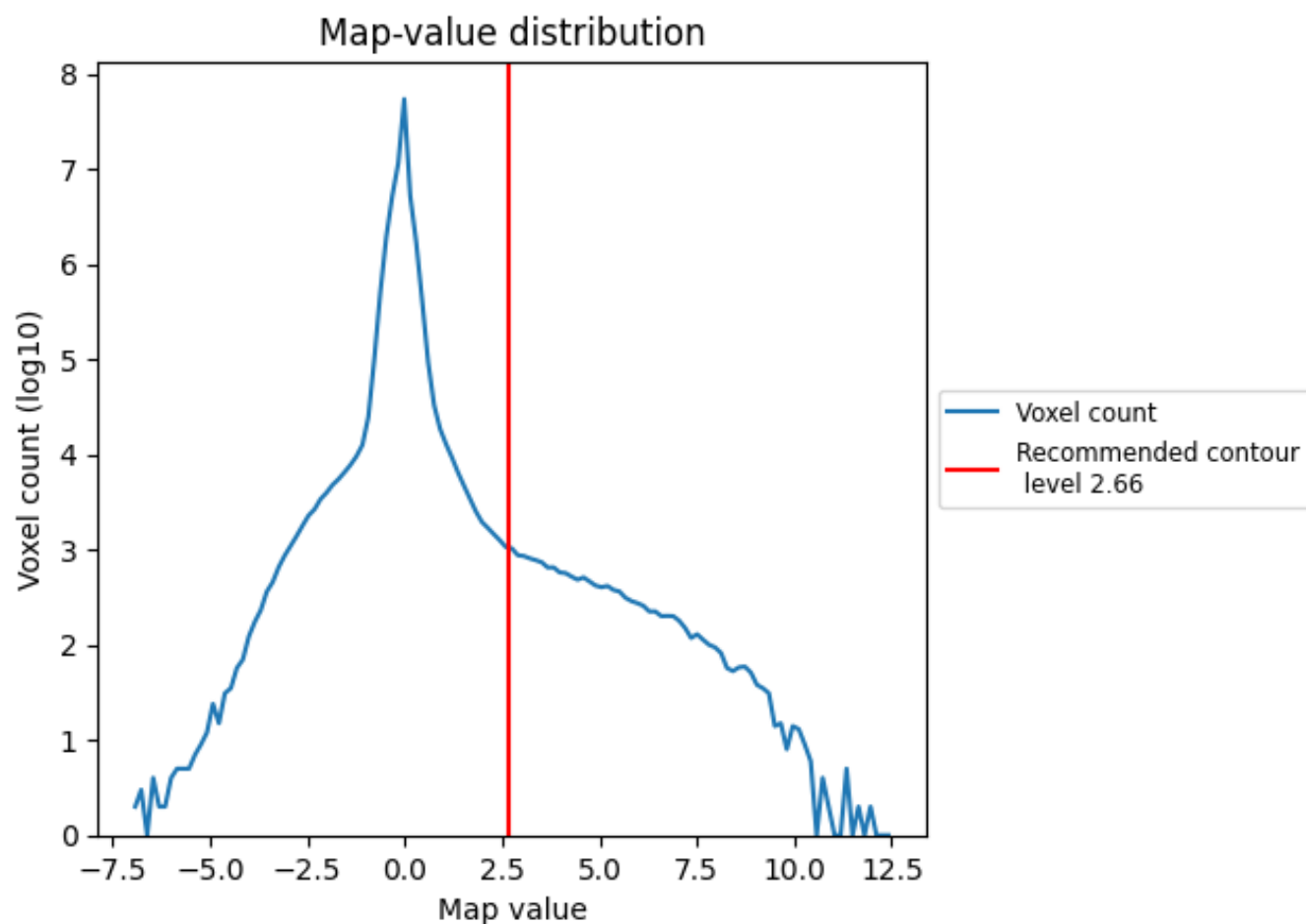
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

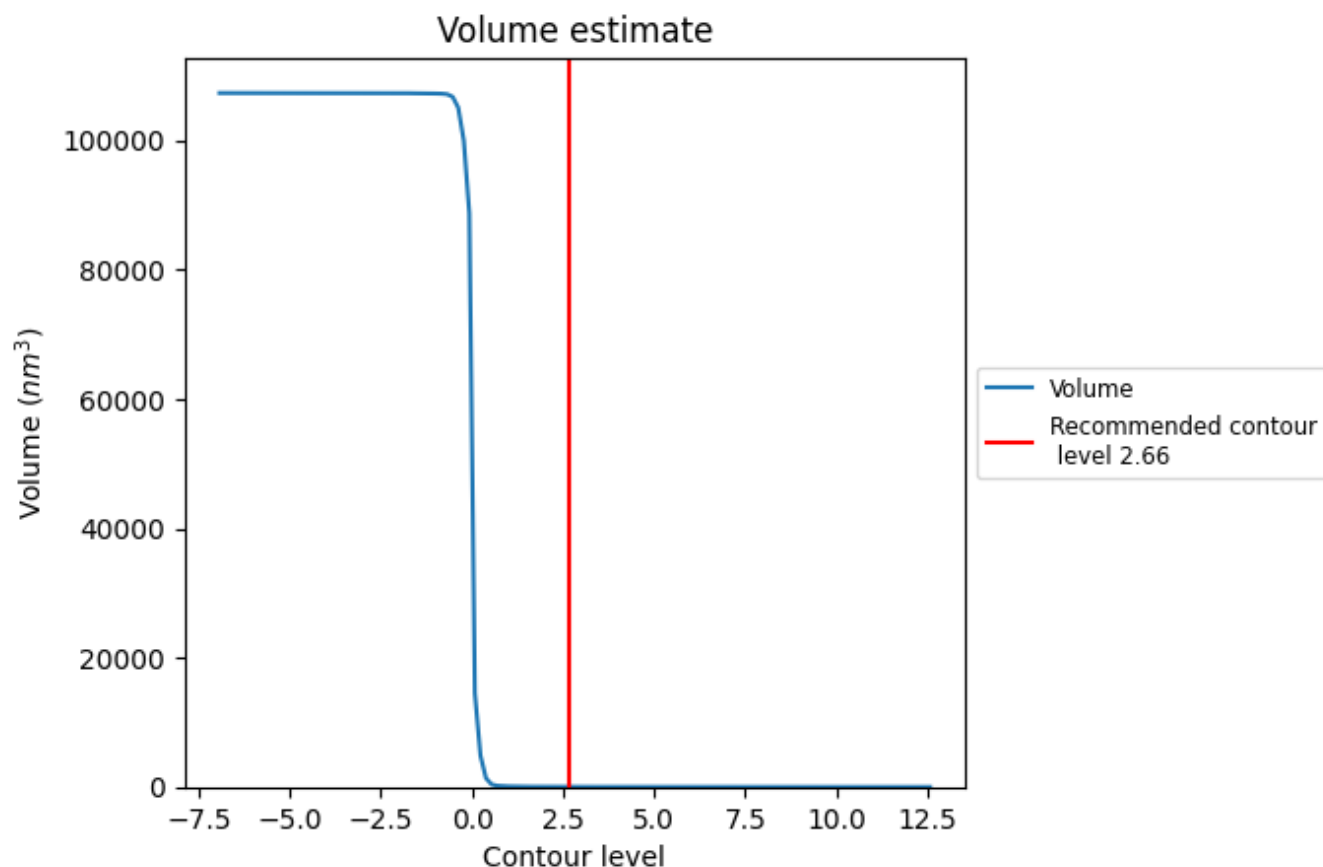
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

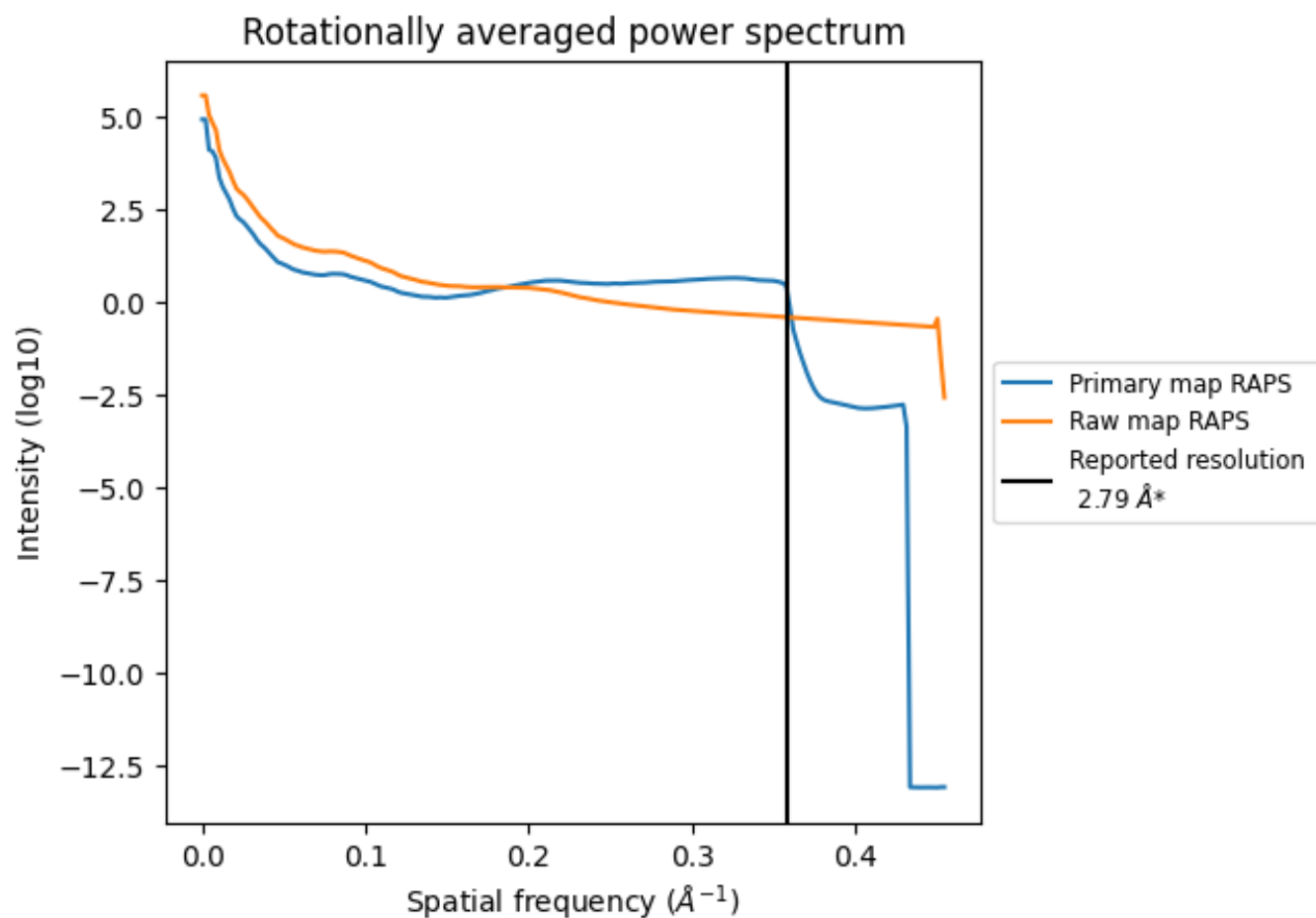
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 21 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 ⓘ

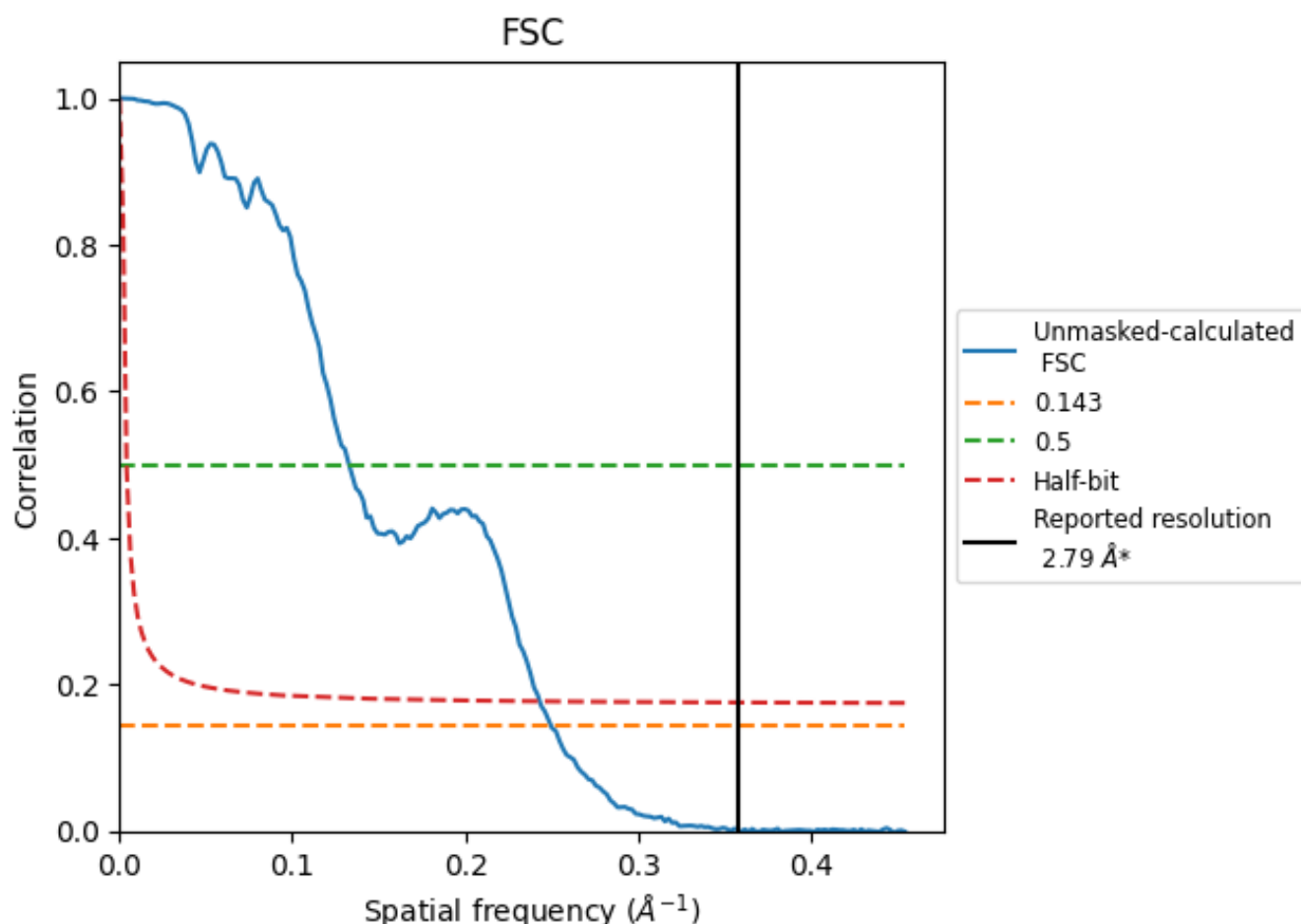


*Reported resolution corresponds to spatial frequency of 0.358 Å⁻¹

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 0.358 Å⁻¹

8.2 Resolution estimates [i](#)

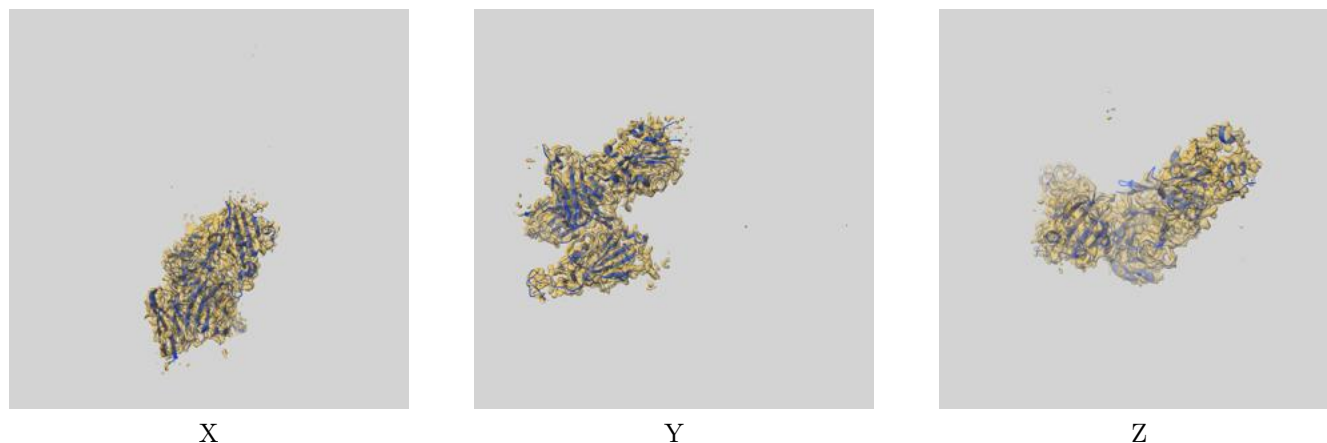
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.00	7.53	4.11

*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 4.00 differs from the reported value 2.79 by more than 10 %

9 Map-model fit [i](#)

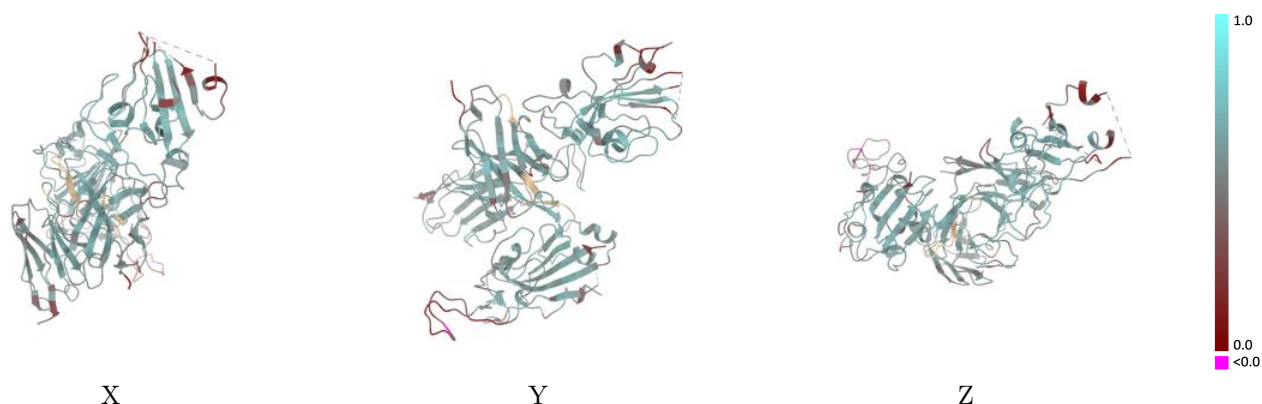
This section contains information regarding the fit between EMDB map EMD-41374 and PDB model 8TM1. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



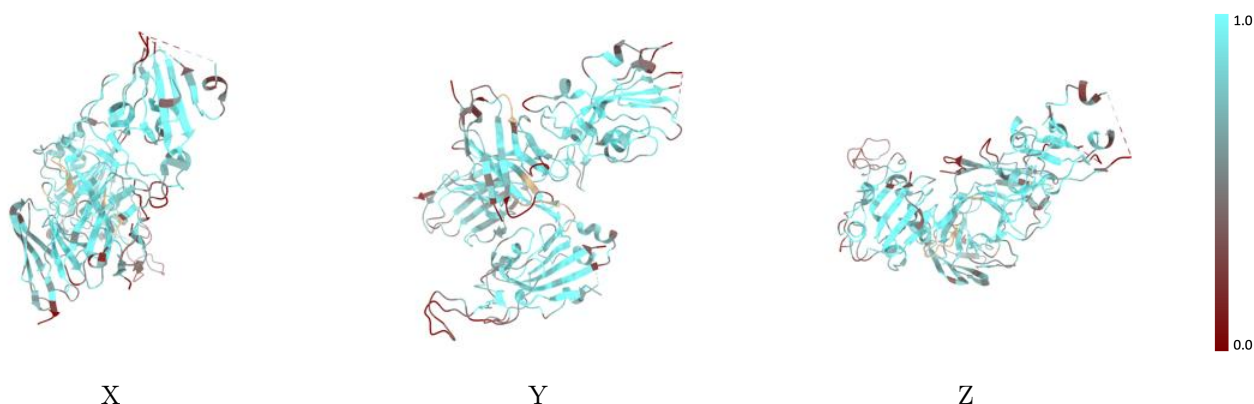
The images above show the 3D surface view of the map at the recommended contour level 2.66 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



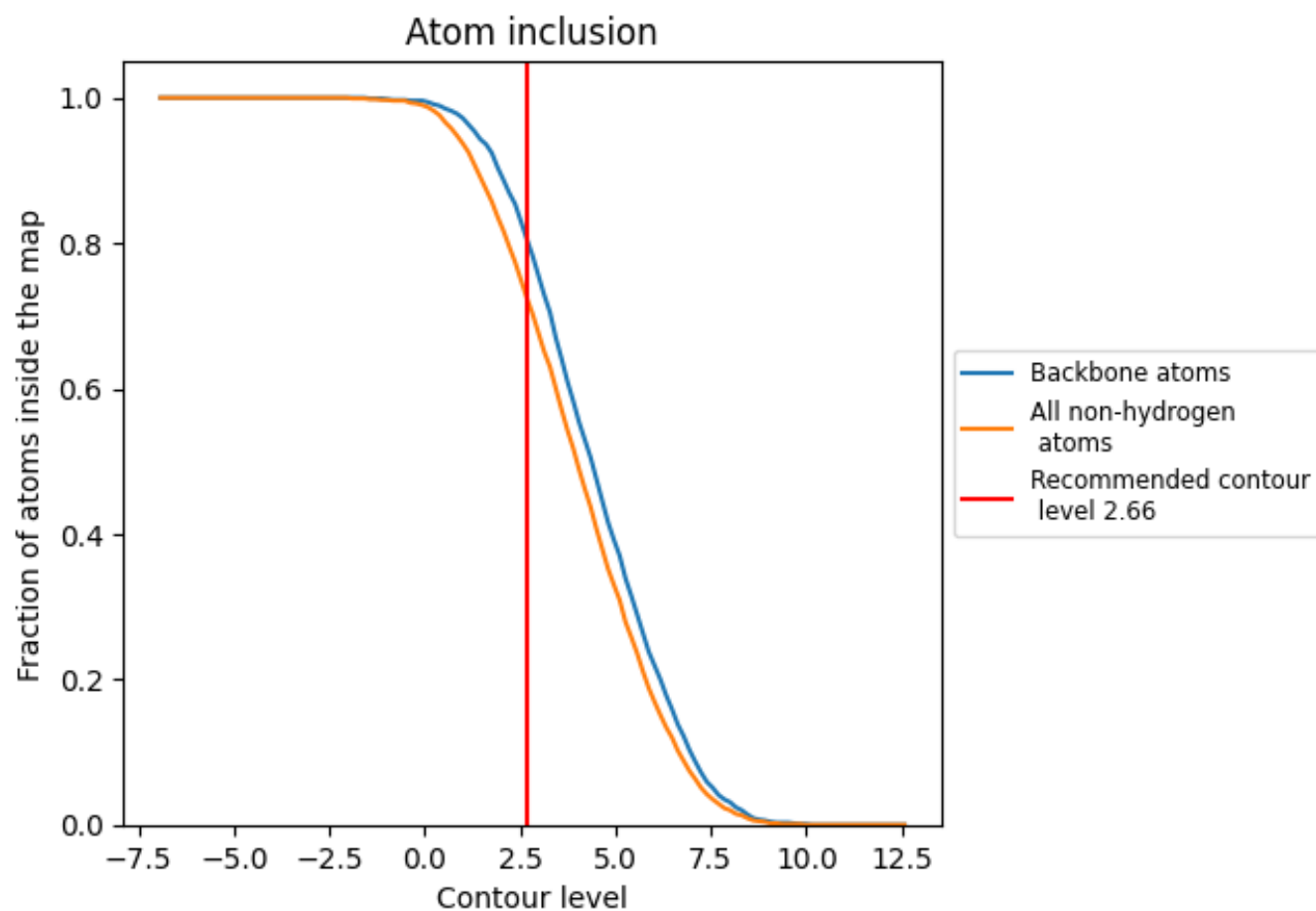
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.66).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (2.66) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7270	<div></div> 0.5430
A	<div></div> 0.7000	<div></div> 0.5160
B	<div></div> 0.7650	<div></div> 0.5570
H	<div></div> 0.7120	<div></div> 0.5560
L	<div></div> 0.7300	<div></div> 0.5530

