



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 03:24 PM UTC

PDB ID : 9QKS / pdb_00009qks
EMDB ID : EMD-53220
Title : B subtilis Type VIIb Core Unit (T7bCU) + DUF
Authors : Oka, G.U.; Fronzes, R.
Deposited on : 2025-03-20
Resolution : 3.80 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:

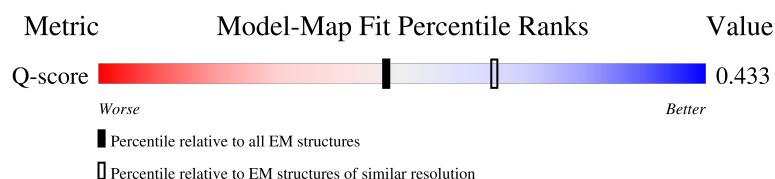
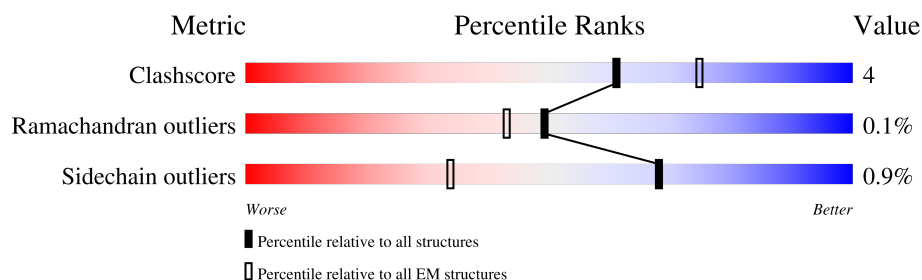
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	81	14% 85% 11% ..
2	C	459	6% 44% 52%
2	D	459	7% 44% 52%
3	G	1265	10% 25% 72%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	1265	9% 39% 5% 55%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11940 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 ESX secretion system protein YukD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	79	Total	C	N	O	S	0	0
			638	406	110	118	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P71071
A	0	GLY	-	expression tag	UNP P71071

- Molecule 2 is a protein called ESX secretion system protein YukC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	221	Total	C	N	O	S	0	0
			1814	1177	296	340	1		
2	D	221	Total	C	N	O	S	0	0
			1814	1177	296	340	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	452	ASP	-	expression tag	UNP P71070
C	453	TYR	-	expression tag	UNP P71070
C	454	LYS	-	expression tag	UNP P71070
C	455	ASP	-	expression tag	UNP P71070
C	456	ASP	-	expression tag	UNP P71070
C	457	ASP	-	expression tag	UNP P71070
C	458	ASP	-	expression tag	UNP P71070
C	459	LYS	-	expression tag	UNP P71070
D	452	ASP	-	expression tag	UNP P71070
D	453	TYR	-	expression tag	UNP P71070
D	454	LYS	-	expression tag	UNP P71070
D	455	ASP	-	expression tag	UNP P71070
D	456	ASP	-	expression tag	UNP P71070

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	457	ASP	-	expression tag	UNP P71070
D	458	ASP	-	expression tag	UNP P71070
D	459	LYS	-	expression tag	UNP P71070

- Molecule 3 is a protein called ESX secretion system protein YukB, Green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	356	Total	C	N	O	S	0	0
			3018	1915	532	562	9		
3	H	564	Total	C	N	O	S	0	0
			4656	2959	795	890	12		

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP C0SPA7
G	2	LEU	-	expression tag	UNP C0SPA7
G	3	PRO	-	expression tag	UNP C0SPA7
G	4	PHE	-	expression tag	UNP C0SPA7
G	5	GLY	-	expression tag	UNP C0SPA7
G	6	ARG	-	expression tag	UNP C0SPA7
G	7	LYS	-	expression tag	UNP C0SPA7
G	8	GLY	-	expression tag	UNP C0SPA7
G	9	VAL	-	expression tag	UNP C0SPA7
G	10	ARG	-	expression tag	UNP C0SPA7
G	11	HIS	-	expression tag	UNP C0SPA7
G	12	LEU	-	expression tag	UNP C0SPA7
G	974	GLY	-	linker	UNP C0SPA7
G	975	ALA	-	linker	UNP C0SPA7
G	976	GLY	-	linker	UNP C0SPA7
G	977	GLY	-	linker	UNP C0SPA7
G	978	LEU	-	linker	UNP C0SPA7
G	979	VAL	-	linker	UNP C0SPA7
G	980	PRO	-	linker	UNP C0SPA7
G	981	ARG	-	linker	UNP C0SPA7
G	982	GLY	-	linker	UNP C0SPA7
G	983	SER	-	linker	UNP C0SPA7
G	984	GLY	-	linker	UNP C0SPA7
G	985	GLY	-	linker	UNP C0SPA7
G	986	SER	-	linker	UNP C0SPA7
G	987	GLY	-	linker	UNP C0SPA7
G	988	SER	-	linker	UNP C0SPA7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	989	VAL	-	linker	UNP C0SPA7
G	990	ASP	-	linker	UNP C0SPA7
G	991	SER	-	linker	UNP C0SPA7
G	992	THR	-	linker	UNP C0SPA7
G	993	GLU	-	linker	UNP C0SPA7
G	994	SER	-	linker	UNP C0SPA7
G	1018	ARG	SER	conflict	UNP P42212
G	1027	ASN	TYR	conflict	UNP P42212
G	1052	LEU	PHE	conflict	UNP P42212
G	1053	THR	SER	conflict	UNP P42212
G	1087	THR	PHE	conflict	UNP P42212
G	1093	THR	ASN	conflict	UNP P42212
G	1141	THR	MET	conflict	UNP P42212
G	1151	ALA	VAL	conflict	UNP P42212
G	1159	VAL	ILE	conflict	UNP P42212
G	1194	LYS	ALA	conflict	UNP P42212
G	1219	GLY	-	expression tag	UNP P42212
G	1220	GLY	-	expression tag	UNP P42212
G	1221	SER	-	expression tag	UNP P42212
G	1222	GLY	-	expression tag	UNP P42212
G	1223	GLY	-	expression tag	UNP P42212
G	1224	SER	-	expression tag	UNP P42212
G	1225	GLY	-	expression tag	UNP P42212
G	1226	SER	-	expression tag	UNP P42212
G	1227	ARG	-	expression tag	UNP P42212
G	1228	GLY	-	expression tag	UNP P42212
G	1229	ARG	-	expression tag	UNP P42212
G	1230	SER	-	expression tag	UNP P42212
G	1231	GLY	-	expression tag	UNP P42212
G	1232	SER	-	expression tag	UNP P42212
G	1233	GLY	-	expression tag	UNP P42212
G	1234	SER	-	expression tag	UNP P42212
G	1235	ALA	-	expression tag	UNP P42212
G	1236	TRP	-	expression tag	UNP P42212
G	1237	SER	-	expression tag	UNP P42212
G	1238	HIS	-	expression tag	UNP P42212
G	1239	PRO	-	expression tag	UNP P42212
G	1240	GLN	-	expression tag	UNP P42212
G	1241	PHE	-	expression tag	UNP P42212
G	1242	GLU	-	expression tag	UNP P42212
G	1243	LYS	-	expression tag	UNP P42212
G	1244	GLY	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	1245	GLY	-	expression tag	UNP P42212
G	1246	GLY	-	expression tag	UNP P42212
G	1247	SER	-	expression tag	UNP P42212
G	1248	GLY	-	expression tag	UNP P42212
G	1249	GLY	-	expression tag	UNP P42212
G	1250	GLY	-	expression tag	UNP P42212
G	1251	SER	-	expression tag	UNP P42212
G	1252	GLY	-	expression tag	UNP P42212
G	1253	GLY	-	expression tag	UNP P42212
G	1254	SER	-	expression tag	UNP P42212
G	1255	ALA	-	expression tag	UNP P42212
G	1256	TRP	-	expression tag	UNP P42212
G	1257	SER	-	expression tag	UNP P42212
G	1258	HIS	-	expression tag	UNP P42212
G	1259	PRO	-	expression tag	UNP P42212
G	1260	GLN	-	expression tag	UNP P42212
G	1261	PHE	-	expression tag	UNP P42212
G	1262	GLU	-	expression tag	UNP P42212
G	1263	LYS	-	expression tag	UNP P42212
G	1264	LYS	-	expression tag	UNP P42212
G	1265	GLY	-	expression tag	UNP P42212
H	1	MET	-	initiating methionine	UNP C0SPA7
H	2	LEU	-	expression tag	UNP C0SPA7
H	3	PRO	-	expression tag	UNP C0SPA7
H	4	PHE	-	expression tag	UNP C0SPA7
H	5	GLY	-	expression tag	UNP C0SPA7
H	6	ARG	-	expression tag	UNP C0SPA7
H	7	LYS	-	expression tag	UNP C0SPA7
H	8	GLY	-	expression tag	UNP C0SPA7
H	9	VAL	-	expression tag	UNP C0SPA7
H	10	ARG	-	expression tag	UNP C0SPA7
H	11	HIS	-	expression tag	UNP C0SPA7
H	12	LEU	-	expression tag	UNP C0SPA7
H	974	GLY	-	linker	UNP C0SPA7
H	975	ALA	-	linker	UNP C0SPA7
H	976	GLY	-	linker	UNP C0SPA7
H	977	GLY	-	linker	UNP C0SPA7
H	978	LEU	-	linker	UNP C0SPA7
H	979	VAL	-	linker	UNP C0SPA7
H	980	PRO	-	linker	UNP C0SPA7
H	981	ARG	-	linker	UNP C0SPA7
H	982	GLY	-	linker	UNP C0SPA7

Continued on next page...

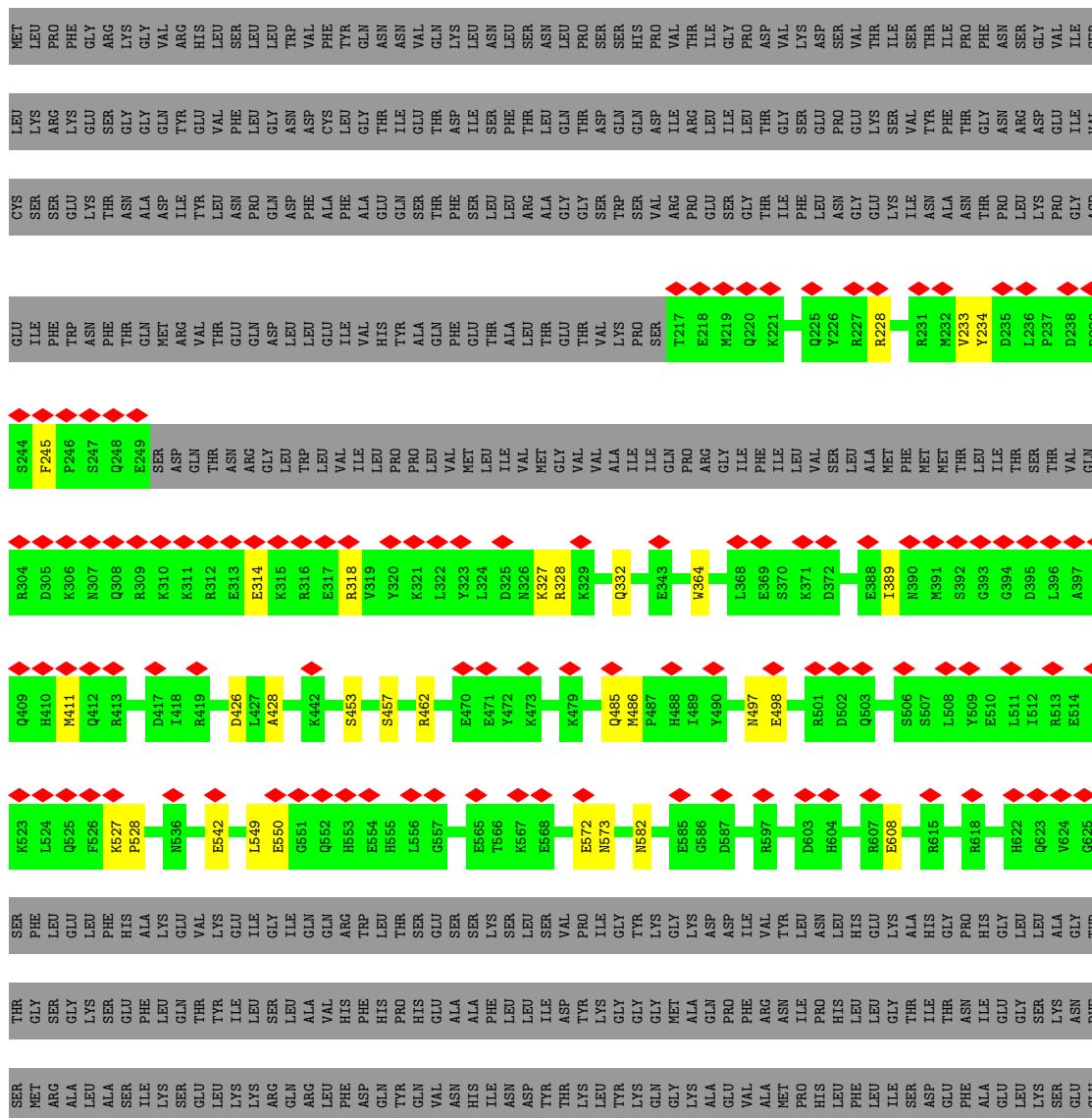
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	983	SER	-	linker	UNP C0SPA7
H	984	GLY	-	linker	UNP C0SPA7
H	985	GLY	-	linker	UNP C0SPA7
H	986	SER	-	linker	UNP C0SPA7
H	987	GLY	-	linker	UNP C0SPA7
H	988	SER	-	linker	UNP C0SPA7
H	989	VAL	-	linker	UNP C0SPA7
H	990	ASP	-	linker	UNP C0SPA7
H	991	SER	-	linker	UNP C0SPA7
H	992	THR	-	linker	UNP C0SPA7
H	993	GLU	-	linker	UNP C0SPA7
H	994	SER	-	linker	UNP C0SPA7
H	1018	ARG	SER	conflict	UNP P42212
H	1027	ASN	TYR	conflict	UNP P42212
H	1052	LEU	PHE	conflict	UNP P42212
H	1053	THR	SER	conflict	UNP P42212
H	1087	THR	PHE	conflict	UNP P42212
H	1093	THR	ASN	conflict	UNP P42212
H	1141	THR	MET	conflict	UNP P42212
H	1151	ALA	VAL	conflict	UNP P42212
H	1159	VAL	ILE	conflict	UNP P42212
H	1194	LYS	ALA	conflict	UNP P42212
H	1219	GLY	-	expression tag	UNP P42212
H	1220	GLY	-	expression tag	UNP P42212
H	1221	SER	-	expression tag	UNP P42212
H	1222	GLY	-	expression tag	UNP P42212
H	1223	GLY	-	expression tag	UNP P42212
H	1224	SER	-	expression tag	UNP P42212
H	1225	GLY	-	expression tag	UNP P42212
H	1226	SER	-	expression tag	UNP P42212
H	1227	ARG	-	expression tag	UNP P42212
H	1228	GLY	-	expression tag	UNP P42212
H	1229	ARG	-	expression tag	UNP P42212
H	1230	SER	-	expression tag	UNP P42212
H	1231	GLY	-	expression tag	UNP P42212
H	1232	SER	-	expression tag	UNP P42212
H	1233	GLY	-	expression tag	UNP P42212
H	1234	SER	-	expression tag	UNP P42212
H	1235	ALA	-	expression tag	UNP P42212
H	1236	TRP	-	expression tag	UNP P42212
H	1237	SER	-	expression tag	UNP P42212
H	1238	HIS	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	1239	PRO	-	expression tag	UNP P42212
H	1240	GLN	-	expression tag	UNP P42212
H	1241	PHE	-	expression tag	UNP P42212
H	1242	GLU	-	expression tag	UNP P42212
H	1243	LYS	-	expression tag	UNP P42212
H	1244	GLY	-	expression tag	UNP P42212
H	1245	GLY	-	expression tag	UNP P42212
H	1246	GLY	-	expression tag	UNP P42212
H	1247	SER	-	expression tag	UNP P42212
H	1248	GLY	-	expression tag	UNP P42212
H	1249	GLY	-	expression tag	UNP P42212
H	1250	GLY	-	expression tag	UNP P42212
H	1251	SER	-	expression tag	UNP P42212
H	1252	GLY	-	expression tag	UNP P42212
H	1253	GLY	-	expression tag	UNP P42212
H	1254	SER	-	expression tag	UNP P42212
H	1255	ALA	-	expression tag	UNP P42212
H	1256	TRP	-	expression tag	UNP P42212
H	1257	SER	-	expression tag	UNP P42212
H	1258	HIS	-	expression tag	UNP P42212
H	1259	PRO	-	expression tag	UNP P42212
H	1260	GLN	-	expression tag	UNP P42212
H	1261	PHE	-	expression tag	UNP P42212
H	1262	GLU	-	expression tag	UNP P42212
H	1263	LYS	-	expression tag	UNP P42212
H	1264	LYS	-	expression tag	UNP P42212
H	1265	GLY	-	expression tag	UNP P42212





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	303198	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.596	Depositor
Minimum map value	-0.247	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	360.0, 360.0, 360.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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	0.17	0/652	0.35	0/880
2	C	0.16	0/1856	0.32	0/2511
2	D	0.16	0/1856	0.32	0/2511
3	G	0.16	0/3084	0.35	0/4146
3	H	0.17	0/4756	0.35	0/6425
All	All	0.17	0/12204	0.34	0/16473

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	A	638	0	635	7	0
2	C	1814	0	1802	21	0
2	D	1814	0	1802	12	0
3	G	3018	0	2972	20	0
3	H	4656	0	4576	45	0
All	All	11940	0	11787	104	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 4.

All (104) 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:C:6:LYS:HA	2:C:10:GLU:OE1	1.68	0.93
2:C:101:ASN:OD1	2:C:102:LEU:N	2.10	0.85
2:D:10:GLU:N	2:D:10:GLU:OE2	2.12	0.81
3:G:550:GLU:O	3:G:573:ASN:ND2	2.19	0.75
3:H:142:GLN:OE1	3:H:142:GLN:N	2.18	0.75
2:C:112:GLU:OE2	2:C:112:GLU:N	2.20	0.74
2:C:7:SER:OG	2:C:10:GLU:HG3	1.87	0.74
2:D:18:GLU:N	2:D:18:GLU:OE2	2.20	0.74
2:C:131:GLU:N	2:C:131:GLU:OE1	2.20	0.74
3:G:403:ASP:OD1	3:G:407:LYS:NZ	2.21	0.73
3:H:82:ILE:HG21	3:H:101:LEU:HD13	1.74	0.69
3:G:542:GLU:N	3:G:542:GLU:OE2	2.26	0.69
3:G:498:GLU:N	3:G:498:GLU:OE1	2.27	0.68
2:D:101:ASN:OD1	2:D:102:LEU:N	2.27	0.67
2:D:134:PRO:O	2:D:136:TYR:N	2.28	0.66
3:H:426:ASP:OD2	3:H:427:LEU:N	2.29	0.66
2:C:7:SER:H	2:C:10:GLU:CD	2.04	0.65
2:C:11:ASN:OD1	2:C:12:GLN:N	2.32	0.62
3:H:320:TYR:CD2	3:H:404:LEU:HD23	2.35	0.62
2:C:6:LYS:CA	2:C:10:GLU:OE1	2.47	0.59
3:H:307:ASN:OD1	3:H:311:LYS:NZ	2.21	0.57
3:G:314:GLU:OE2	3:G:318:ARG:NE	2.37	0.57
2:C:162:GLU:N	2:C:162:GLU:OE2	2.38	0.57
3:H:107:GLU:N	3:H:107:GLU:OE1	2.38	0.56
1:A:36:GLN:O	1:A:36:GLN:NE2	2.33	0.56
3:H:577:LEU:HD23	3:H:589:LEU:HD11	1.89	0.55
2:C:11:ASN:OD1	2:C:11:ASN:C	2.50	0.55
1:A:13:ASN:O	1:A:13:ASN:OD1	2.25	0.54
2:C:7:SER:N	2:C:10:GLU:OE1	2.40	0.54
3:H:166:ASN:ND2	3:H:180:ASP:OD1	2.39	0.54
3:H:541:SER:OG	3:H:542:GLU:OE2	2.25	0.53
3:H:42:ASP:OD1	3:H:43:VAL:N	2.43	0.52
2:D:174:SER:OG	2:D:175:ALA:N	2.42	0.52
3:H:82:ILE:HG21	3:H:101:LEU:CD1	2.37	0.52
1:A:46:GLU:OE1	3:H:50:SER:OG	2.25	0.52
3:G:328:ARG:HA	3:G:411:MET:HE3	1.92	0.51
3:H:512:ILE:HD12	3:H:558:ILE:HD11	1.93	0.51
2:D:216:ASN:OD1	2:D:216:ASN:C	2.53	0.51
3:G:228:ARG:NH2	3:G:364:TRP:O	2.45	0.49
3:H:340:GLN:OE1	3:H:340:GLN:C	2.56	0.49
3:H:212:THR:OG1	3:H:213:VAL:N	2.44	0.49
2:D:106:ASN:ND2	2:D:136:TYR:O	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:76:ASN:OD1	3:H:76:ASN:N	2.40	0.49
2:C:14:GLU:N	2:C:14:GLU:OE1	2.47	0.48
2:C:60:ASP:CG	2:C:61:GLU:OE1	2.57	0.48
3:G:497:ASN:ND2	3:G:498:GLU:OE1	2.46	0.48
3:H:245:PHE:CE1	3:H:405:MET:SD	3.06	0.48
2:C:101:ASN:OD1	2:C:101:ASN:C	2.57	0.47
3:G:245:PHE:CD2	3:G:405:MET:HE1	2.50	0.47
3:G:233:VAL:HG12	3:G:234:TYR:N	2.29	0.47
3:G:486:MET:HE3	3:G:486:MET:HA	1.97	0.47
3:H:516:ASP:OD2	3:H:516:ASP:C	2.58	0.46
2:C:101:ASN:OD1	2:C:102:LEU:HD23	2.16	0.46
3:H:596:VAL:CG1	3:H:597:ARG:N	2.79	0.46
2:C:82:ASP:OD2	2:C:84:LYS:N	2.49	0.45
2:D:44:ILE:O	2:D:47:ILE:HG22	2.16	0.45
3:H:245:PHE:C	3:H:245:PHE:CD1	2.94	0.45
3:H:352:MET:HE1	3:H:451:GLN:HG2	1.99	0.45
3:H:82:ILE:CG2	3:H:101:LEU:HD13	2.44	0.45
2:C:31:GLU:OE1	2:C:31:GLU:N	2.43	0.45
3:G:582:ASN:OD1	3:G:582:ASN:N	2.50	0.45
1:A:41:SER:OG	1:A:42:MET:N	2.50	0.44
3:H:325:ASP:OD1	3:H:328:ARG:NH1	2.45	0.44
3:H:571:SER:OG	3:H:573:ASN:OD1	2.16	0.44
3:H:78:CYS:O	3:H:79:LEU:HD22	2.18	0.44
1:A:31:ILE:HD13	1:A:78:ILE:HD13	1.98	0.44
2:D:133:ILE:HB	2:D:134:PRO:CD	2.47	0.44
3:H:246:PRO:HD3	3:H:320:TYR:CZ	2.52	0.44
3:H:577:LEU:HD23	3:H:589:LEU:CD1	2.47	0.44
3:H:498:GLU:OE2	3:H:501:ARG:NH2	2.46	0.43
3:H:571:SER:OG	3:H:572:GLU:N	2.51	0.43
3:H:91:GLN:CD	3:H:91:GLN:C	2.85	0.43
3:H:74:LEU:O	3:H:74:LEU:HD23	2.19	0.43
3:H:562:VAL:HG12	3:H:563:ALA:N	2.34	0.43
2:C:169:GLU:OE1	2:C:169:GLU:N	2.49	0.43
2:C:60:ASP:OD1	2:C:60:ASP:C	2.62	0.42
2:C:184:GLU:OE1	2:C:184:GLU:HA	2.18	0.42
3:G:426:ASP:OD2	3:G:428:ALA:N	2.52	0.42
3:H:469:GLU:OE2	3:H:469:GLU:N	2.36	0.42
3:G:242:SER:O	3:G:327:LYS:NZ	2.51	0.42
3:G:572:GLU:OE2	3:G:572:GLU:HA	2.20	0.42
3:H:320:TYR:CG	3:H:404:LEU:HD23	2.55	0.42
2:C:12:GLN:C	2:C:13:LEU:HD23	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:231:ARG:NE	3:H:365:GLU:OE2	2.52	0.42
2:D:47:ILE:HD11	2:D:127:TYR:CZ	2.54	0.42
3:H:366:LYS:NZ	3:H:372:ASP:O	2.40	0.42
1:A:38:GLN:O	1:A:39:SER:OG	2.34	0.41
3:H:578:VAL:HG12	3:H:579:ARG:N	2.35	0.41
3:G:332:GLN:C	3:G:332:GLN:CD	2.88	0.41
3:H:486:MET:HE2	3:H:486:MET:HA	2.03	0.41
2:D:17:ALA:C	2:D:18:GLU:OE2	2.62	0.41
3:G:608:GLU:HA	3:G:608:GLU:OE2	2.21	0.41
3:G:389:ILE:O	3:G:389:ILE:HG23	2.21	0.41
3:H:396:LEU:C	3:H:396:LEU:HD23	2.46	0.40
3:H:467:PHE:N	3:H:467:PHE:CD1	2.90	0.40
3:H:546:LEU:HD23	3:H:546:LEU:HA	1.95	0.40
3:H:596:VAL:HG12	3:H:597:ARG:N	2.36	0.40
3:H:101:LEU:HD12	3:H:101:LEU:N	2.36	0.40
3:H:174:THR:HG22	3:H:175:PRO:O	2.22	0.40
1:A:41:SER:C	1:A:42:MET:HG3	2.46	0.40
3:G:462:ARG:NH1	3:G:485:GLN:O	2.54	0.40
3:G:527:LYS:HB3	3:G:528:PRO:HD3	2.03	0.40
3:H:406:GLU:OE1	3:H:407:LYS:N	2.55	0.40
2:D:76:ARG:NH1	2:D:76:ARG:HG3	2.35	0.40

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	77/81 (95%)	70 (91%)	6 (8%)	1 (1%)	9	38
2	C	219/459 (48%)	210 (96%)	9 (4%)	0	100	100
2	D	219/459 (48%)	208 (95%)	11 (5%)	0	100	100
3	G	352/1265 (28%)	335 (95%)	17 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	556/1265 (44%)	532 (96%)	24 (4%)	0	100	100
All	All	1423/3529 (40%)	1355 (95%)	67 (5%)	1 (0%)	49	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	MET

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	72/73 (99%)	71 (99%)	1 (1%)	59	70
2	C	192/406 (47%)	191 (100%)	1 (0%)	81	81
2	D	192/406 (47%)	191 (100%)	1 (0%)	81	81
3	G	334/1112 (30%)	331 (99%)	3 (1%)	70	74
3	H	523/1112 (47%)	517 (99%)	6 (1%)	65	73
All	All	1313/3109 (42%)	1301 (99%)	12 (1%)	68	74

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
2	C	133	ILE
2	D	7	SER
3	G	453	SER
3	G	457	SER
3	G	549	LEU
3	H	96	ASP
3	H	195	ASP
3	H	367	SER
3	H	373	TYR
3	H	488	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	919	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
2	C	126	HIS
2	D	209	HIS
2	D	218	GLN
3	G	220	GLN
3	G	326	ASN
3	G	555	HIS
3	G	584	HIS
3	H	22	ASN
3	H	133	ASN
3	H	398	ASN
3	H	446	HIS
3	H	468	HIS
3	H	553	HIS

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.

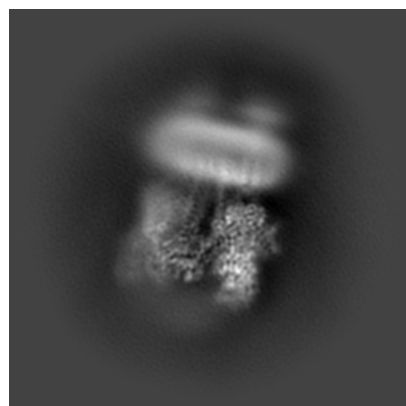
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53220. These allow visual inspection of the internal detail of the map and identification of artifacts.

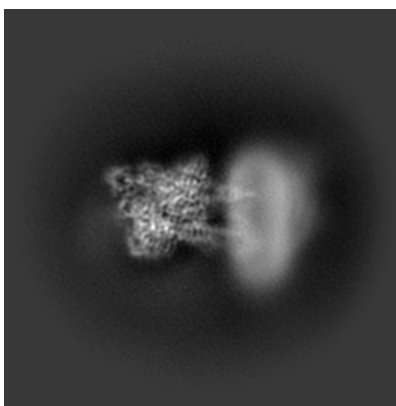
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

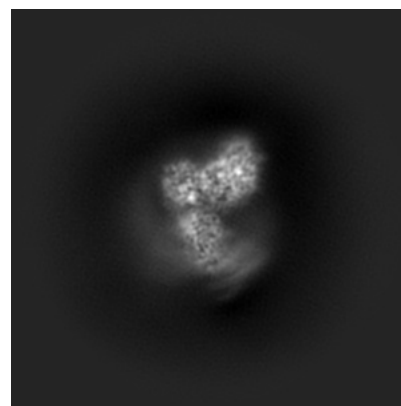
6.1.1 Primary map



X

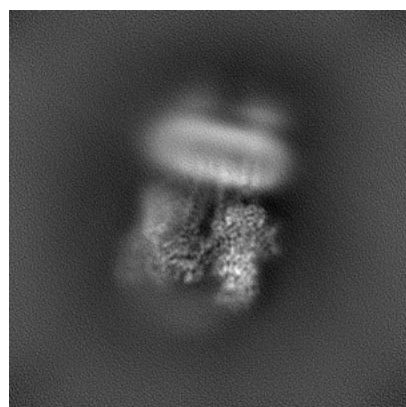


Y

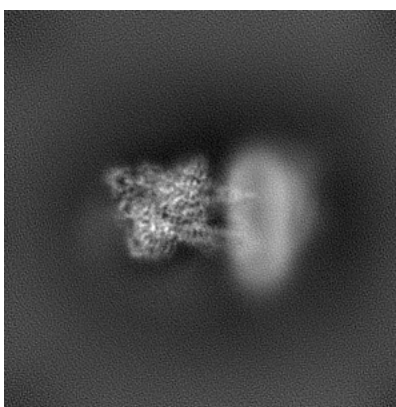


Z

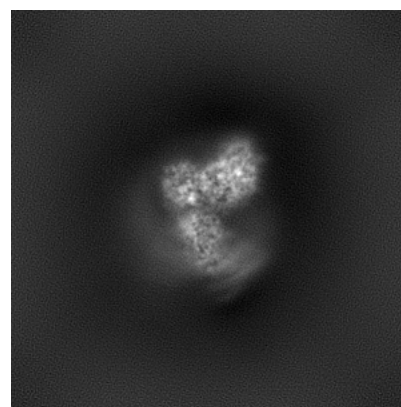
6.1.2 Raw map



X



Y

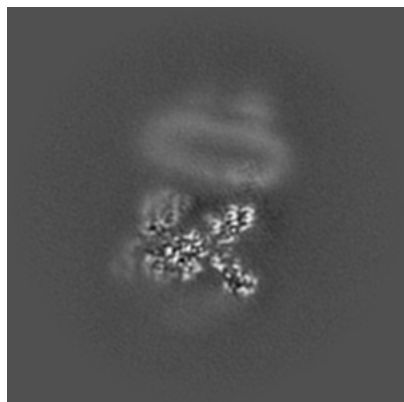


Z

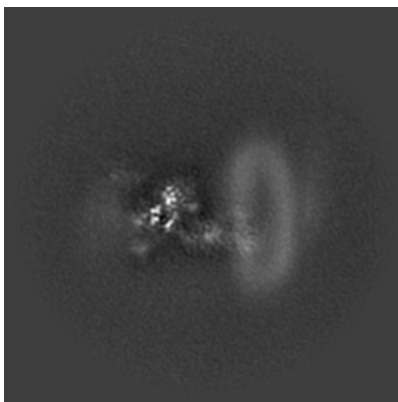
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

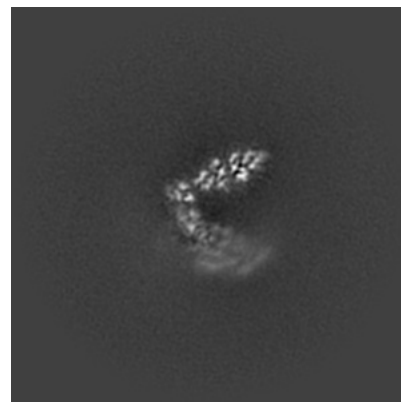
6.2.1 Primary map



X Index: 150

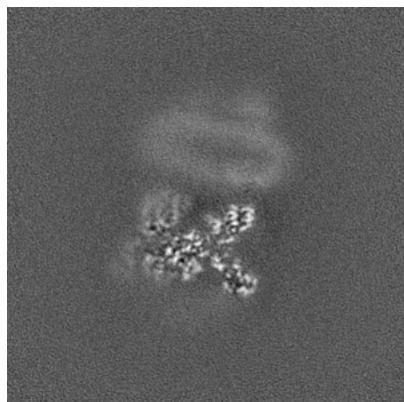


Y Index: 150

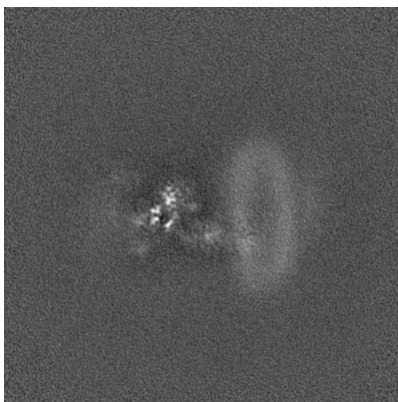


Z Index: 150

6.2.2 Raw map



X Index: 150



Y Index: 150

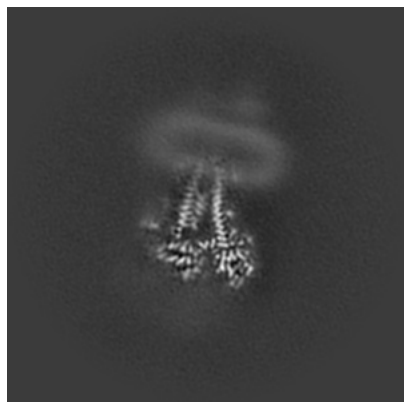


Z Index: 150

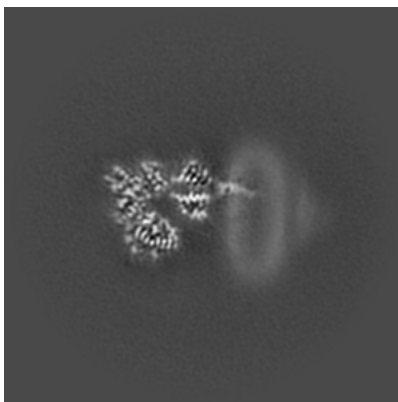
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

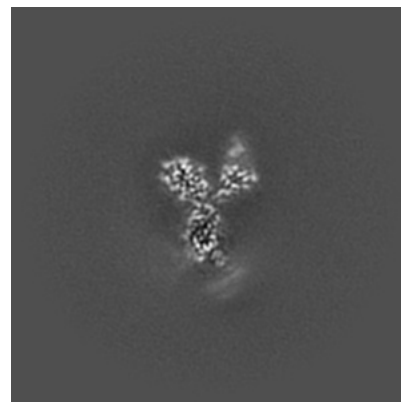
6.3.1 Primary map



X Index: 135

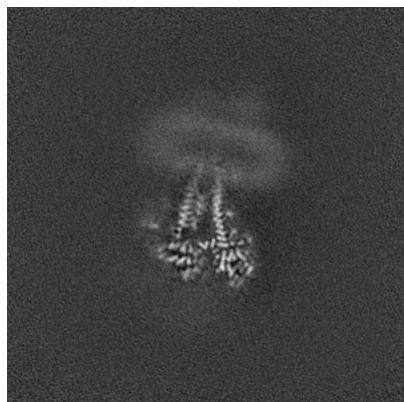


Y Index: 175

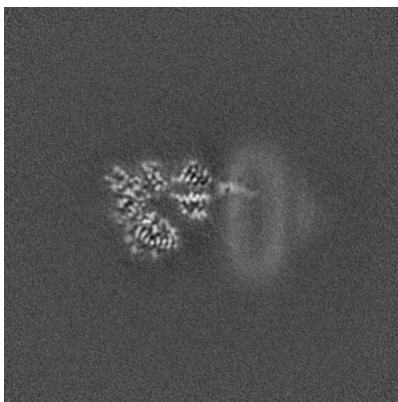


Z Index: 115

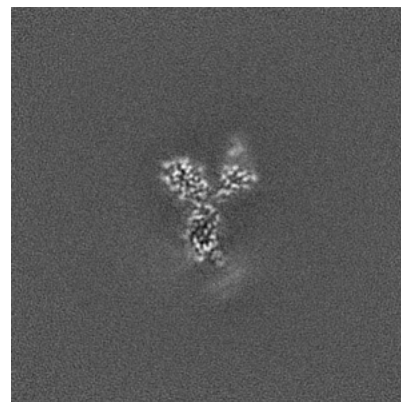
6.3.2 Raw map



X Index: 135



Y Index: 175



Z Index: 115

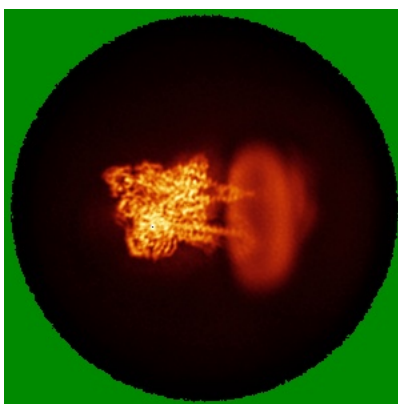
The images above show the largest variance slices of the map in three orthogonal directions.

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

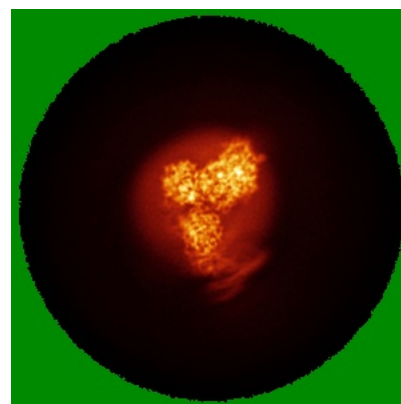
6.4.1 Primary map



X

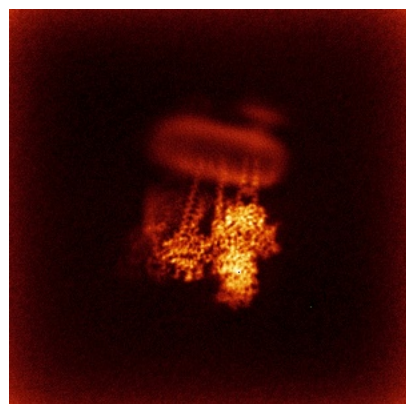


Y

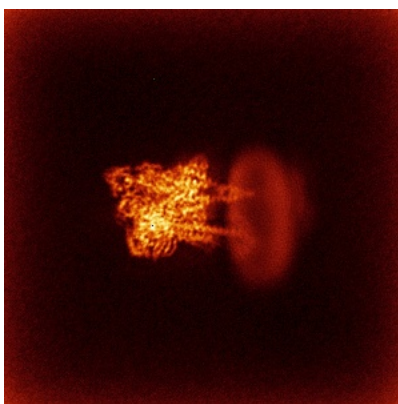


Z

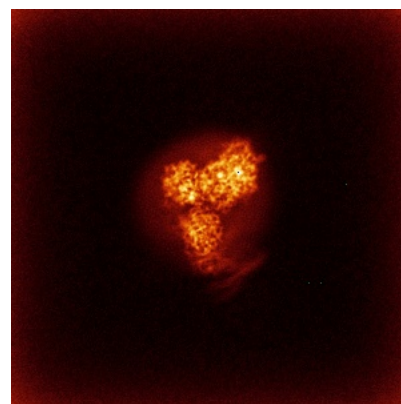
6.4.2 Raw map



X



Y

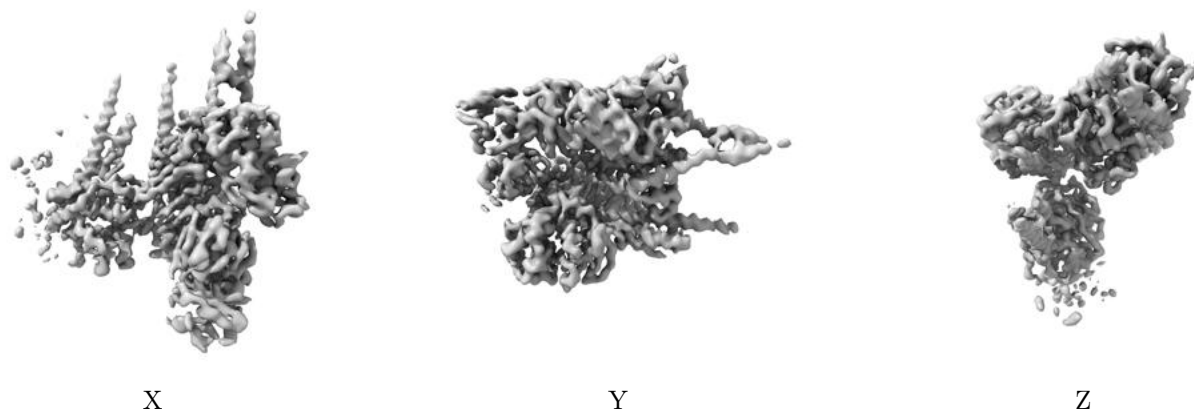


Z

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 0.2. 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.

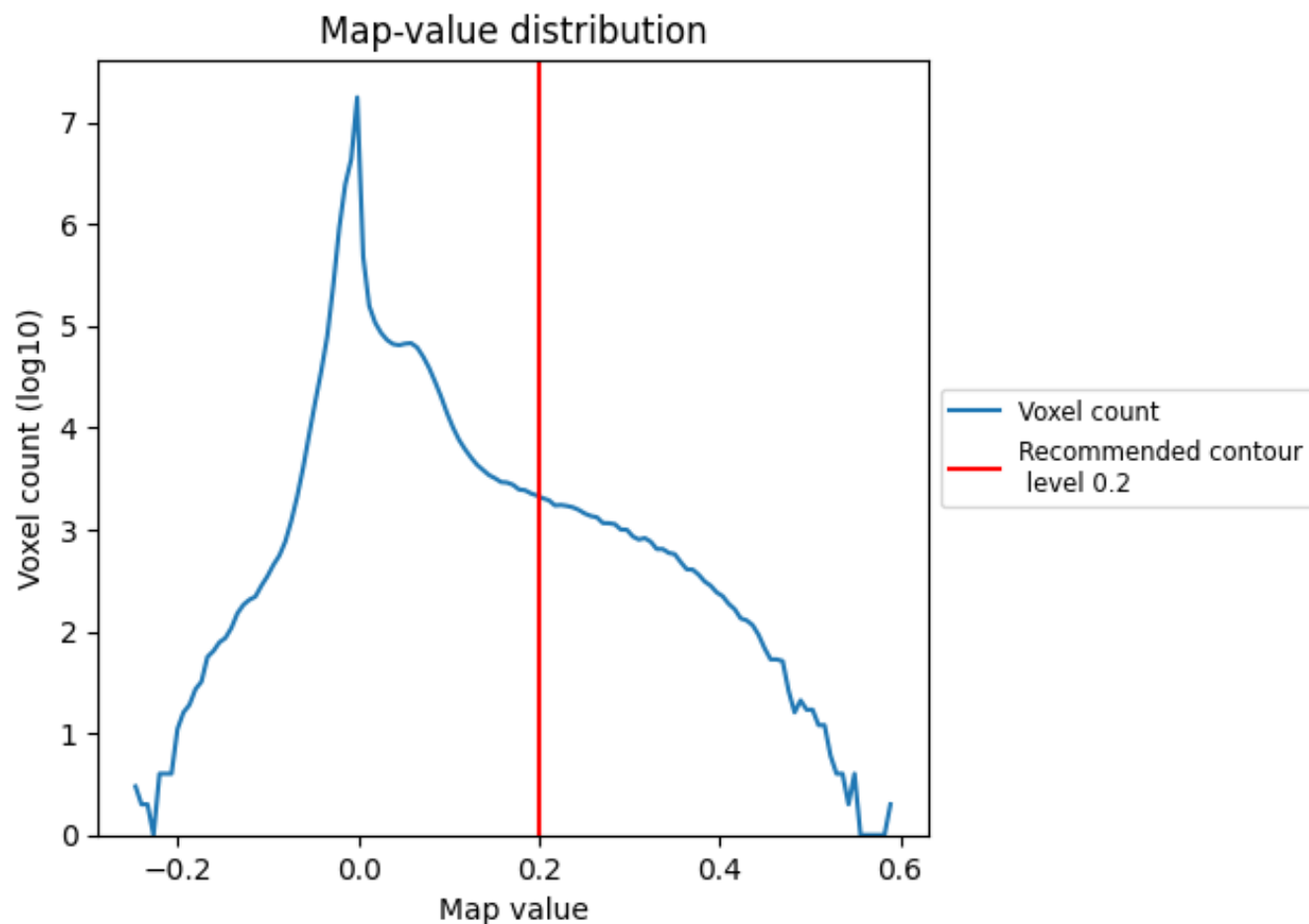
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

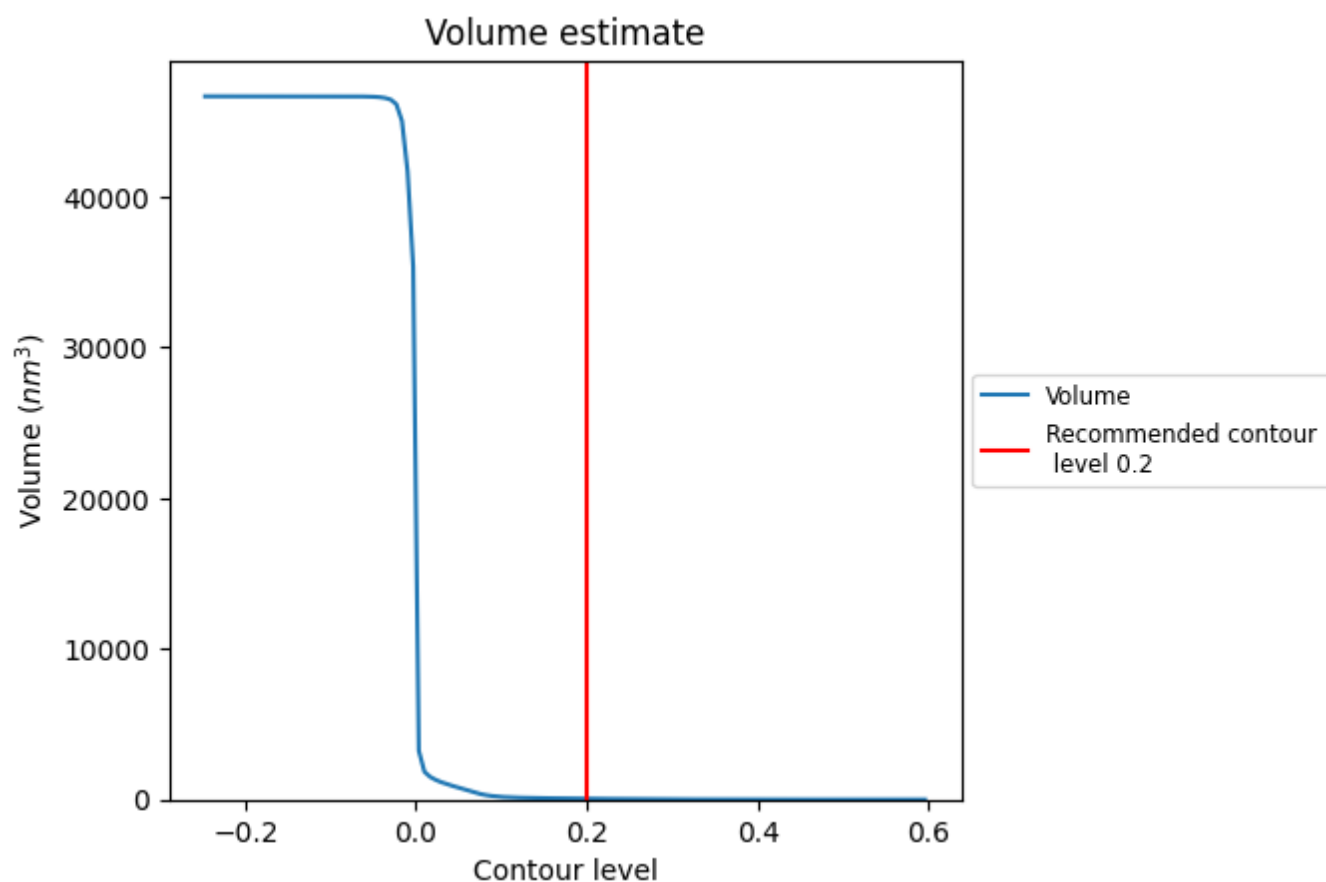
This section contains the results of statistical analysis of the map.

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.

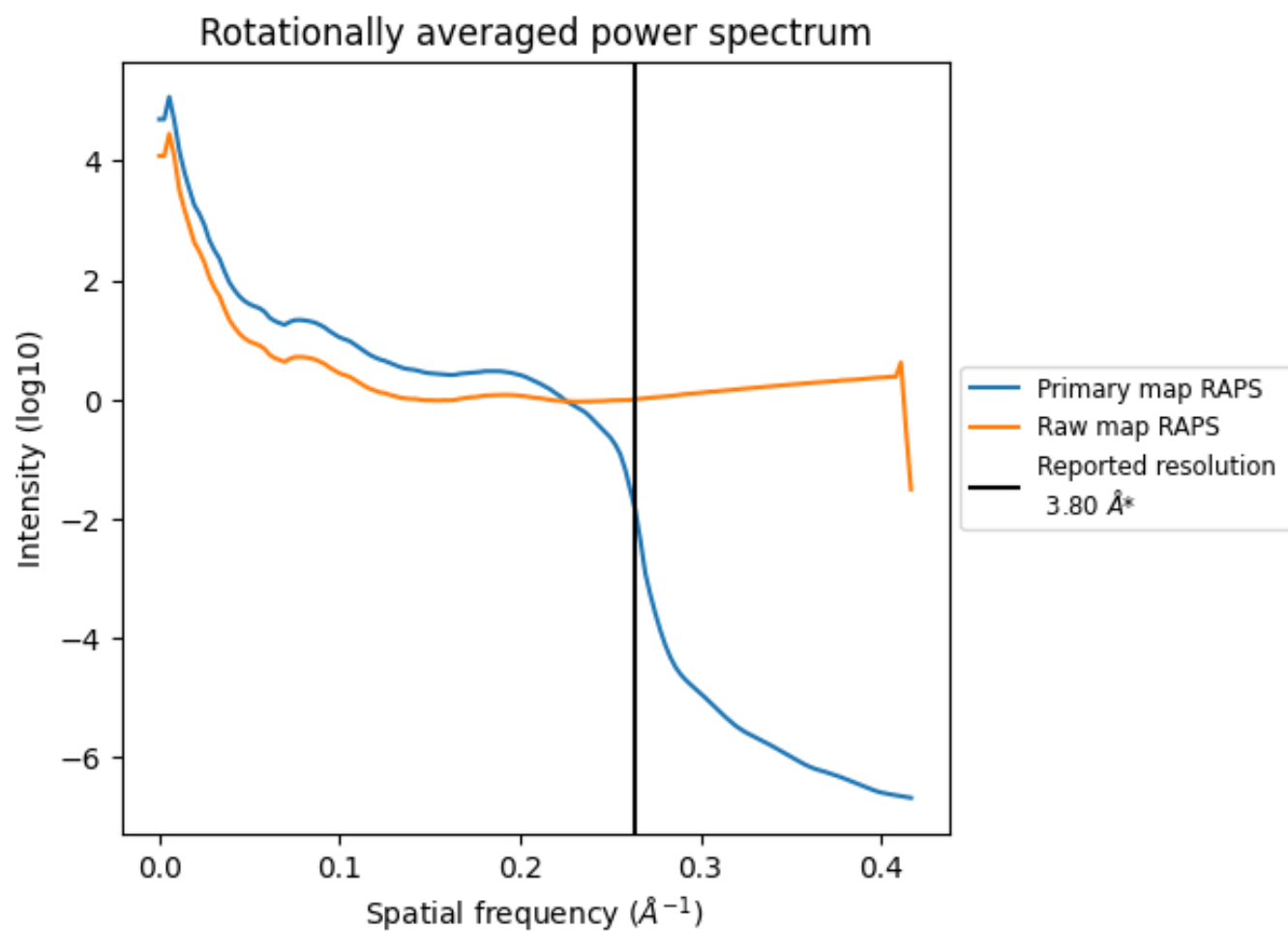
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 57 nm³; this corresponds to an approximate mass of 51 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 ⓘ

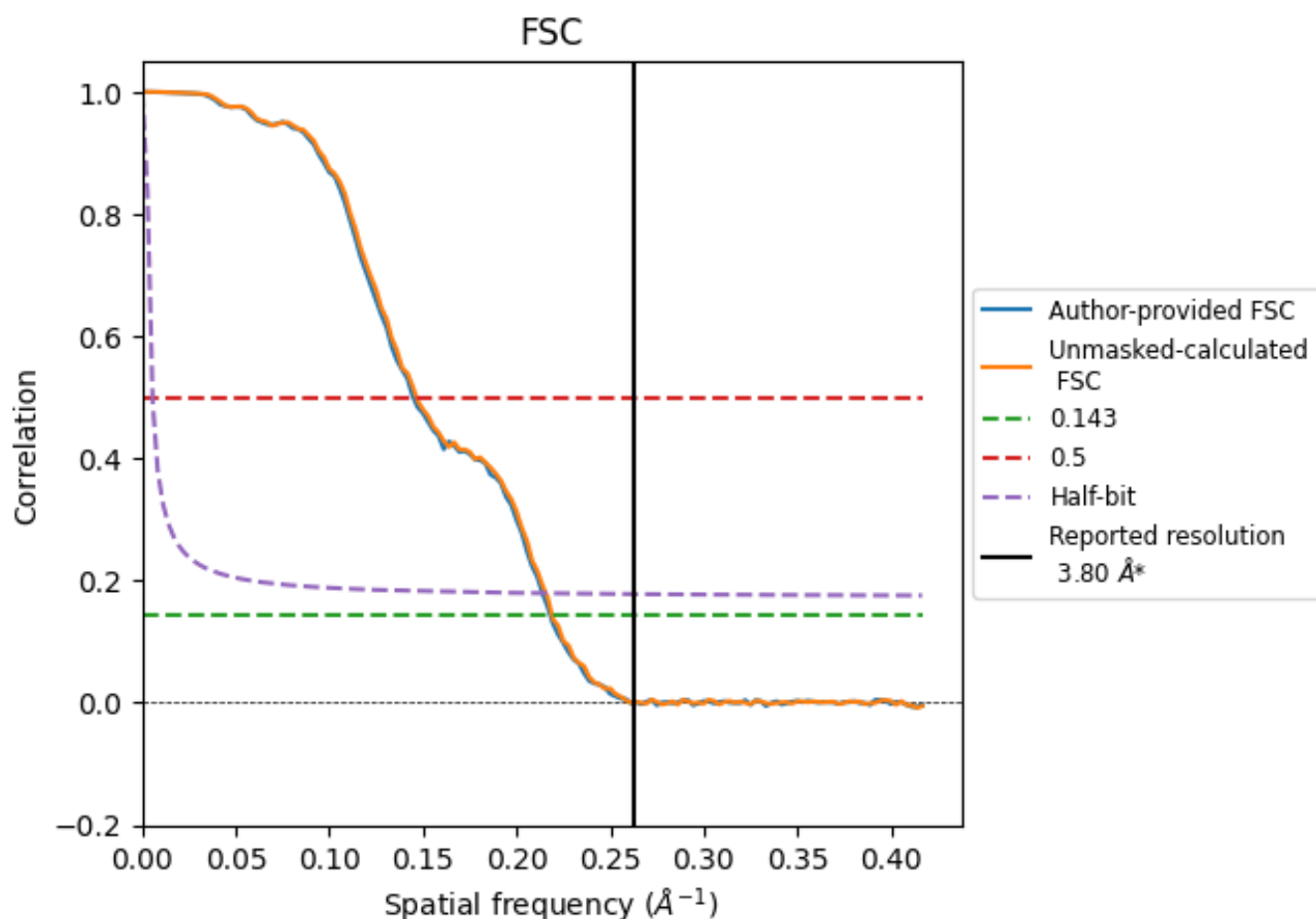


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	4.59	6.91	4.68
Unmasked-calculated*	4.57	6.83	4.64

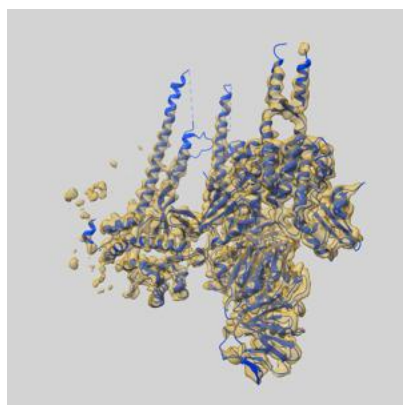
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.59 differs from the reported value 3.8 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.57 differs from the reported value 3.8 by more than 10 %

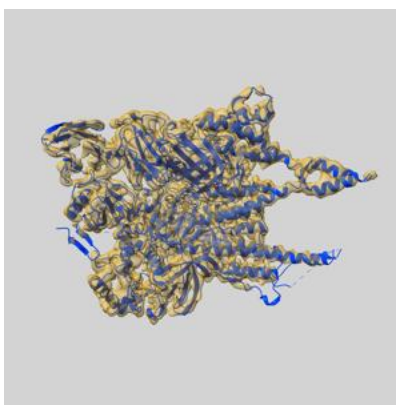
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53220 and PDB model 9QKS. Per-residue inclusion information can be found in section 3 on page 10.

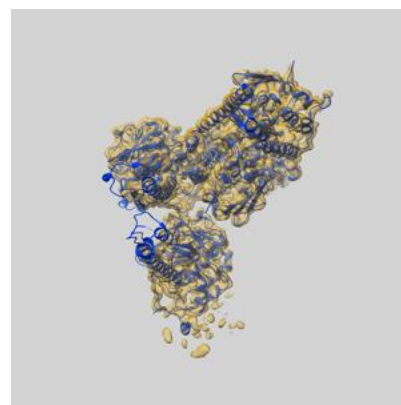
9.1 Map-model overlay [i](#)



X



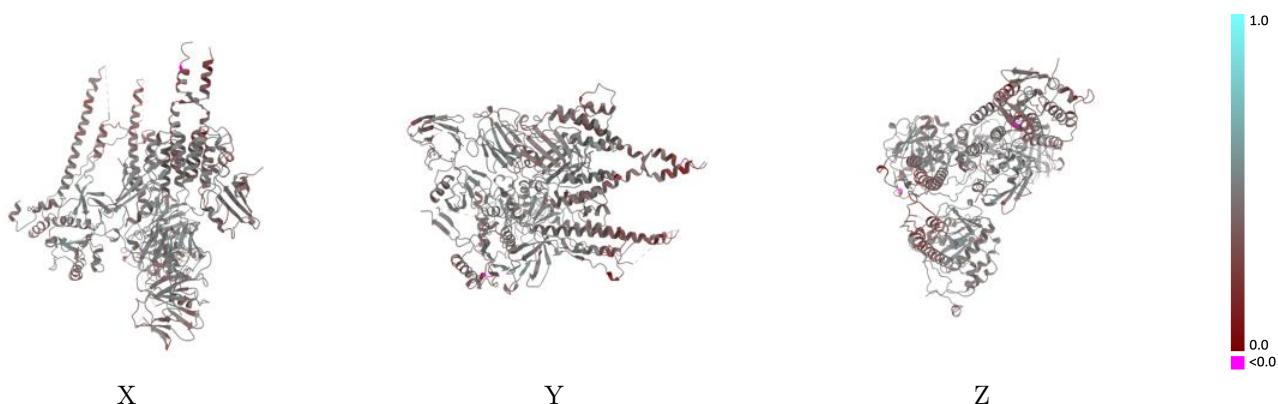
Y



Z

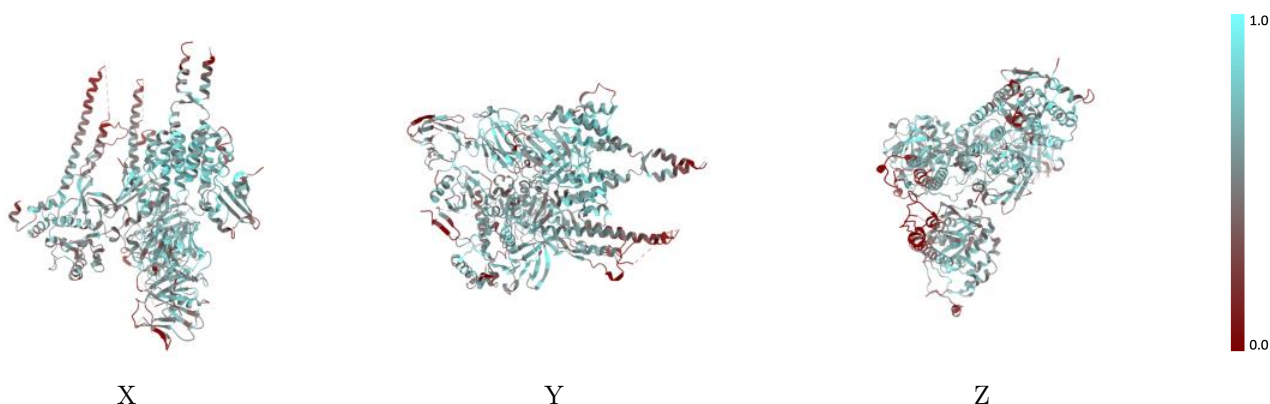
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



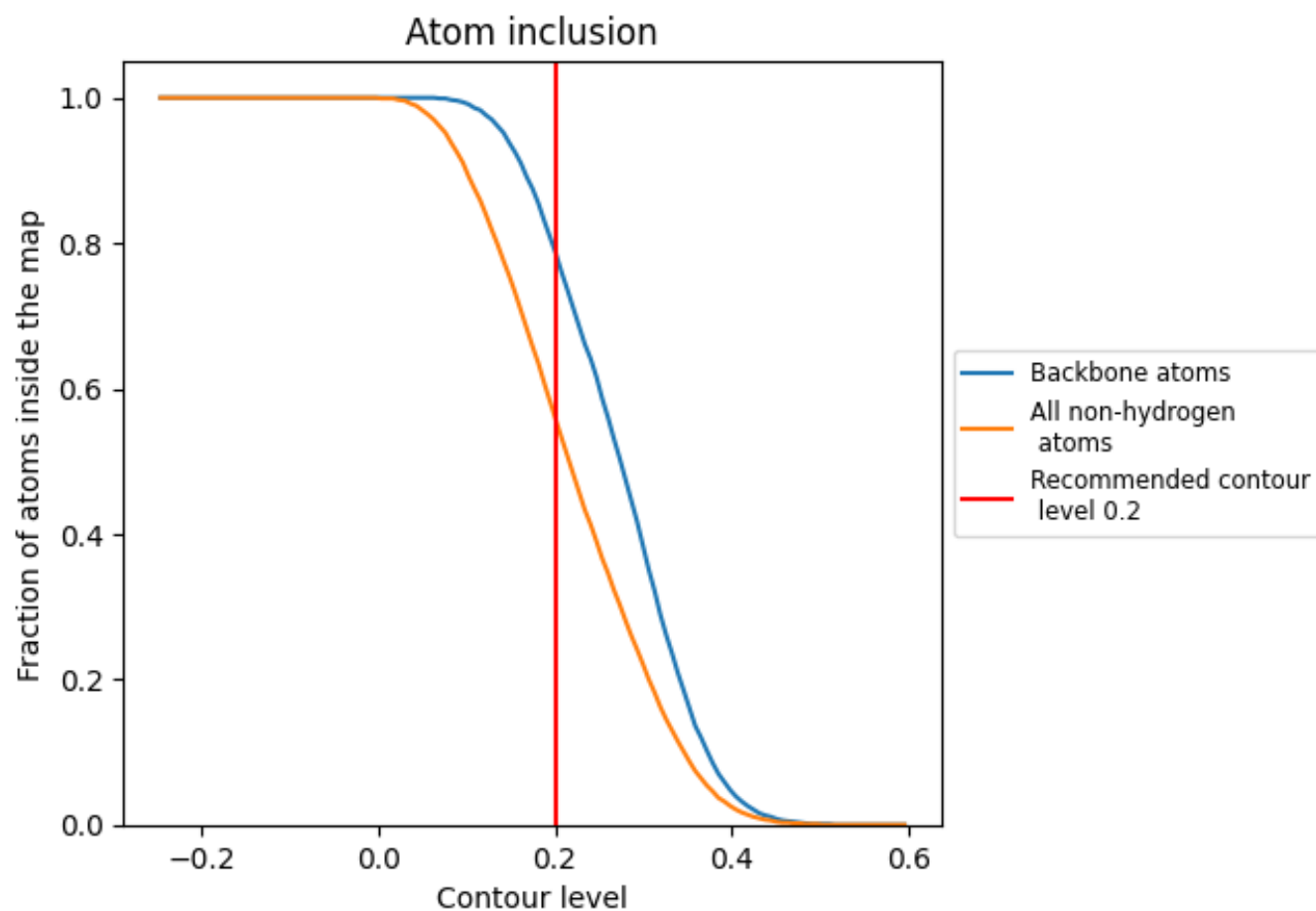
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 56% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5600	0.4330
A	0.5900	0.4590
C	0.6140	0.4190
D	0.6200	0.4430
G	0.4640	0.4230
H	0.5750	0.4360

