



Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 01:49 AM JST

PDB ID : 7CXR
EMDB ID : EMD-30495
Title : Cryo-EM structure of human TMEM120A/TACAN
Authors : Yan, Z.; Wu, J.; Ke, M.
Deposited on : 2020-09-02
Resolution : 3.40 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.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

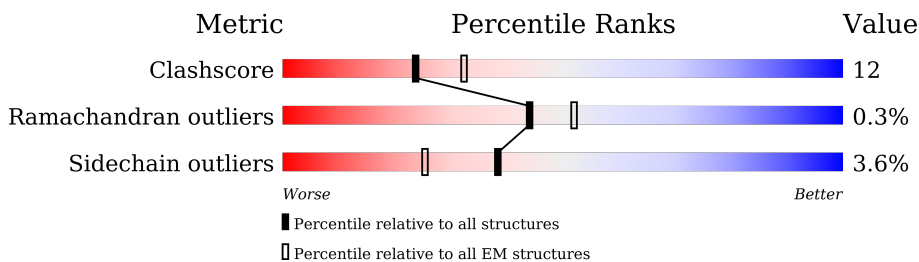
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	625	
1	B	625	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5168 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 MCherry fluorescent protein, Ion channel TACAN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	307	2584	1703	429	438	14	0	0
1	B	307	2584	1703	429	438	14	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-281	MET	-	expression tag	UNP X5DSL3
A	-280	ASP	-	expression tag	UNP X5DSL3
A	-279	TYR	-	expression tag	UNP X5DSL3
A	-278	LYS	-	expression tag	UNP X5DSL3
A	-277	ASP	-	expression tag	UNP X5DSL3
A	-276	ASP	-	expression tag	UNP X5DSL3
A	-275	ASP	-	expression tag	UNP X5DSL3
A	-274	ASP	-	expression tag	UNP X5DSL3
A	-273	LYS	-	expression tag	UNP X5DSL3
A	-272	GLY	-	expression tag	UNP X5DSL3
A	-271	SER	-	expression tag	UNP X5DSL3
A	-270	ASP	-	expression tag	UNP X5DSL3
A	-269	TYR	-	expression tag	UNP X5DSL3
A	-268	LYS	-	expression tag	UNP X5DSL3
A	-267	ASP	-	expression tag	UNP X5DSL3
A	-266	ASP	-	expression tag	UNP X5DSL3
A	-265	ASP	-	expression tag	UNP X5DSL3
A	-264	ASP	-	expression tag	UNP X5DSL3
A	-263	LYS	-	expression tag	UNP X5DSL3
A	-262	GLY	-	expression tag	UNP X5DSL3
A	-261	SER	-	expression tag	UNP X5DSL3
A	-260	ASP	-	expression tag	UNP X5DSL3
A	-259	TYR	-	expression tag	UNP X5DSL3
A	-258	LYS	-	expression tag	UNP X5DSL3
A	-257	ASP	-	expression tag	UNP X5DSL3
A	-256	ASP	-	expression tag	UNP X5DSL3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-255	ASP	-	expression tag	UNP X5DSL3
A	-254	ASP	-	expression tag	UNP X5DSL3
A	-253	LYS	-	expression tag	UNP X5DSL3
A	-252	GLY	-	expression tag	UNP X5DSL3
A	-251	SER	-	expression tag	UNP X5DSL3
A	-250	ASP	-	expression tag	UNP X5DSL3
A	-249	GLU	-	expression tag	UNP X5DSL3
A	-248	VAL	-	expression tag	UNP X5DSL3
A	-247	ASP	-	expression tag	UNP X5DSL3
A	-246	ALA	-	expression tag	UNP X5DSL3
A	-9	LEU	-	linker	UNP X5DSL3
A	-8	GLU	-	linker	UNP X5DSL3
A	-7	VAL	-	linker	UNP X5DSL3
A	-6	LEU	-	linker	UNP X5DSL3
A	-5	PHE	-	linker	UNP X5DSL3
A	-4	GLN	-	linker	UNP X5DSL3
A	-3	GLY	-	linker	UNP X5DSL3
A	-2	PRO	-	linker	UNP X5DSL3
A	-1	GLU	-	linker	UNP X5DSL3
A	0	PHE	-	linker	UNP X5DSL3
B	-281	MET	-	expression tag	UNP X5DSL3
B	-280	ASP	-	expression tag	UNP X5DSL3
B	-279	TYR	-	expression tag	UNP X5DSL3
B	-278	LYS	-	expression tag	UNP X5DSL3
B	-277	ASP	-	expression tag	UNP X5DSL3
B	-276	ASP	-	expression tag	UNP X5DSL3
B	-275	ASP	-	expression tag	UNP X5DSL3
B	-274	ASP	-	expression tag	UNP X5DSL3
B	-273	LYS	-	expression tag	UNP X5DSL3
B	-272	GLY	-	expression tag	UNP X5DSL3
B	-271	SER	-	expression tag	UNP X5DSL3
B	-270	ASP	-	expression tag	UNP X5DSL3
B	-269	TYR	-	expression tag	UNP X5DSL3
B	-268	LYS	-	expression tag	UNP X5DSL3
B	-267	ASP	-	expression tag	UNP X5DSL3
B	-266	ASP	-	expression tag	UNP X5DSL3
B	-265	ASP	-	expression tag	UNP X5DSL3
B	-264	ASP	-	expression tag	UNP X5DSL3
B	-263	LYS	-	expression tag	UNP X5DSL3
B	-262	GLY	-	expression tag	UNP X5DSL3
B	-261	SER	-	expression tag	UNP X5DSL3
B	-260	ASP	-	expression tag	UNP X5DSL3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-259	TYR	-	expression tag	UNP X5DSL3
B	-258	LYS	-	expression tag	UNP X5DSL3
B	-257	ASP	-	expression tag	UNP X5DSL3
B	-256	ASP	-	expression tag	UNP X5DSL3
B	-255	ASP	-	expression tag	UNP X5DSL3
B	-254	ASP	-	expression tag	UNP X5DSL3
B	-253	LYS	-	expression tag	UNP X5DSL3
B	-252	GLY	-	expression tag	UNP X5DSL3
B	-251	SER	-	expression tag	UNP X5DSL3
B	-250	ASP	-	expression tag	UNP X5DSL3
B	-249	GLU	-	expression tag	UNP X5DSL3
B	-248	VAL	-	expression tag	UNP X5DSL3
B	-247	ASP	-	expression tag	UNP X5DSL3
B	-246	ALA	-	expression tag	UNP X5DSL3
B	-9	LEU	-	linker	UNP X5DSL3
B	-8	GLU	-	linker	UNP X5DSL3
B	-7	VAL	-	linker	UNP X5DSL3
B	-6	LEU	-	linker	UNP X5DSL3
B	-5	PHE	-	linker	UNP X5DSL3
B	-4	GLN	-	linker	UNP X5DSL3
B	-3	GLY	-	linker	UNP X5DSL3
B	-2	PRO	-	linker	UNP X5DSL3
B	-1	GLU	-	linker	UNP X5DSL3
B	0	PHE	-	linker	UNP X5DSL3

GLY	SER	THR	ASP	Q21	E84	F195	H309	GLY	THR	ASP	Q21	E84	F195	H309
SER	VAL	MET	ILE	D22	N85	Y198	F314	SER	THR	ILE	D22	N85	Y198	F314
VAL	ASN	GLY	TRP	F23	Q86	W210	L317	THR	GLY	TRP	F23	Q86	W210	L317
ASN	LEU	TRP	GLY	Q24	M87	F219	F318	TRP	GLY	TRP	Q24	M87	F219	F318
LEU	LEU	LEU	HIS	N25	K88	Y329	L319	GLY	TRP	TRP	N25	K88	Y329	L319
HIS	GLY	ASP	ALA	I26	E89	Q222	F323	TRP	ASP	ALA	I26	E89	Q222	F323
GLY	GLY	PHE	SER	T29	R90	S242	F326	ASP	TRP	SER	T29	R90	S242	F326
GLY	GLY	PHE	SER	H30	Q91	G243	R327	TRP	THR	ASP	H30	Q91	G243	R327
GLY	GLY	ILE	ILE	R31	L93	CYS	Y328	THR	THR	ILE	R31	L93	CYS	Y328
GLY	GLY	ARG	ARG	L32	F94	LEU	H330	THR	THR	ARG	L32	F94	LEU	H330
GLY	GLY	TYR	TYR	F33	F95	LEU	H331	THR	THR	TYR	F33	F95	LEU	H331
GLY	GLY	PHE	GLY	R34	D96	ARG	K332	THR	THR	GLY	R34	D96	ARG	K332
GLY	GLY	LYS	LYS	L35	L101	TRP	F333	THR	THR	LYS	L35	L101	TRP	F333
GLY	GLY	TRP	TRP	R36	P102	LEU	H334	THR	THR	TRP	R36	P102	LEU	H334
GLY	GLY	GLY	GLY	L37	K103	ARG	S335	THR	THR	GLY	L37	K103	ARG	S335
GLY	GLY	ALA	ALA	E38	K104	GLY	Q336	THR	THR	ALA	E38	K104	GLY	Q336
GLY	GLY	VAL	VAL	E39	M105	GLY	R337	THR	THR	VAL	E39	M105	GLY	R337
GLY	GLY	ASN	ASN	L40	L109	ARG	H338	THR	THR	ASN	L40	L109	ARG	H338
GLY	GLY	PHE	PHE	L41	V112	HIS	GLY	THR	THR	PHE	L41	V112	HIS	GLY
GLY	GLY	GLY	GLY	K42	L113	THR	SER	THR	THR	GLY	K42	L113	THR	SER
GLY	GLY	GLN	GLN	L43	L116	THR	ASP	THR	THR	GLN	L43	L116	THR	ASP
GLY	GLY	GLY	GLY	Q44	L120	GLY	SER	THR	THR	GLY	Q44	L120	GLY	SER
GLY	GLY	VAL	VAL	N45	L121	GLY	LYS	THR	THR	VAL	N45	L121	GLY	LYS
GLY	GLY	THR	THR	C47	E132	PHE	ASP	THR	THR	THR	C47	E132	PHE	ASP
GLY	GLY	LEU	LEU	T48	L140	TRP	TRP	THR	THR	LEU	T48	L140	TRP	TRP
GLY	GLY	LEU	LEU	I51	L140	TRP	M268	THR	THR	LEU	I51	L140	TRP	TRP
GLY	GLY	LEU	LEU	T52	L140	TRP	L275	THR	THR	LEU	T52	L140	TRP	TRP
GLY	GLY	LEU	LEU	R53	L140	TRP	L276	THR	THR	LEU	R53	L140	TRP	TRP
GLY	GLY	LEU	LEU	Q54	L140	TRP	P277	THR	THR	LEU	Q54	L140	TRP	TRP
GLY	GLY	LEU	LEU	PHE	C151	TRP	Q286	THR	THR	LEU	PHE	C151	TRP	TRP
GLY	GLY	LEU	LEU	K55	R152	TRP	L287	THR	THR	LEU	K55	R152	TRP	TRP
GLY	GLY	LEU	LEU	K56	F153	TRP	F288	THR	THR	LEU	K56	F153	TRP	TRP
GLY	GLY	LEU	LEU	R57	L154	TRP	A290	THR	THR	LEU	R57	L154	TRP	TRP
GLY	GLY	LEU	LEU	L58	R158	TRP	L293	THR	THR	LEU	L58	R158	TRP	TRP
GLY	GLY	LEU	LEU	Q59	M165	TRP	Q298	THR	THR	LEU	Q59	M165	TRP	TRP
GLY	GLY	LEU	LEU	MET	L168	TRP	D299	THR	THR	LEU	MET	L168	TRP	TRP
GLY	GLY	LEU	LEU	E60	V169	TRP	F300	THR	THR	LEU	E60	V169	TRP	TRP
GLY	GLY	LEU	LEU	L61	W170	TRP	C302	THR	THR	LEU	L61	W170	TRP	TRP
GLY	GLY	LEU	LEU	A62	Y171	TRP	K303	THR	THR	LEU	A62	Y171	TRP	TRP
GLY	GLY	LEU	LEU	L66	R178	TRP	Q306	THR	THR	LEU	L66	R178	TRP	TRP
GLY	GLY	LEU	LEU	K66	I183	TRP	V307	THR	THR	LEU	K66	I183	TRP	TRP
GLY	GLY	LEU	LEU	K67	M184	TRP	L308	THR	THR	LEU	K67	M184	TRP	TRP
GLY	GLY	LEU	LEU	C68	M185	TRP		THR	THR	LEU	C68	M185	TRP	TRP
GLY	GLY	LEU	LEU	K69	M188	TRP		THR	THR	LEU	K69	M188	TRP	TRP
GLY	GLY	LEU	LEU	P70	I189	TRP		THR	THR	LEU	P70	I189	TRP	TRP
GLY	GLY	LEU	LEU	S71	K190	TRP		THR	THR	LEU	S71	K190	TRP	TRP
GLY	GLY	LEU	LEU	L72		TRP		THR	THR	LEU	L72		TRP	TRP
GLY	GLY	LEU	LEU	P73		TRP		THR	THR	LEU	P73		TRP	TRP
GLY	GLY	LEU	LEU	A74		TRP		THR	THR	LEU	A74		TRP	TRP
GLY	GLY	LEU	LEU	E75		TRP		THR	THR	LEU	E75		TRP	TRP
GLY	GLY	LEU	LEU	A76		TRP		THR	THR	LEU	A76		TRP	TRP
GLY	GLY	LEU	LEU	E77		TRP		THR	THR	LEU	E77		TRP	TRP
GLY	GLY	LEU	LEU	G78		TRP		THR	THR	LEU	G78		TRP	TRP
GLY	GLY	LEU	LEU	A79		TRP		THR	THR	LEU	A79		TRP	TRP
GLY	GLY	LEU	LEU	A80		TRP		THR	THR	LEU	A80		TRP	TRP
GLY	GLY	LEU	LEU	Q81		TRP		THR	THR	LEU	Q81		TRP	TRP
GLY	GLY	LEU	LEU	E82		TRP		THR	THR	LEU	E82		TRP	TRP
GLY	GLY	LEU	LEU	L83		TRP		THR	THR	LEU	L83		TRP	TRP
GLY	GLY	LEU	LEU			TRP		THR	THR	LEU			TRP	TRP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79080	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.232	Depositor
Minimum map value	-3.326	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	239.14, 239.14, 239.14	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	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	0.41	0/2657	0.49	0/3588
1	B	0.41	0/2657	0.50	0/3588
All	All	0.41	0/5314	0.50	0/7176

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	2584	0	2575	69	0
1	B	2584	0	2575	63	0
All	All	5168	0	5150	125	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 12.

All (125) 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:B:222:GLN:NE2	1:B:289:ASN:OD1	2.20	0.75
1:B:105:ASN:ND2	1:B:116:VAL:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASN:ND2	1:A:116:VAL:O	2.21	0.73
1:A:222:GLN:NE2	1:A:289:ASN:OD1	2.20	0.73
1:A:183:ILE:O	1:A:188:ARG:NH1	2.26	0.69
1:B:183:ILE:O	1:B:188:ARG:NH1	2.26	0.69
1:B:44:GLN:O	1:B:48:THR:HG23	1.97	0.64
1:A:58:LEU:HD11	1:A:91:GLN:HG3	1.80	0.64
1:B:79:ALA:O	1:B:83:LEU:HG	2.01	0.61
1:A:40:LEU:HD12	1:B:40:LEU:HD12	1.82	0.60
1:A:54:GLN:HG2	1:A:94:PHE:CD2	2.37	0.60
1:B:58:LEU:HD11	1:B:91:GLN:HG3	1.84	0.60
1:B:112:VAL:HG12	1:B:113:LEU:HD23	1.84	0.60
1:B:23:PHE:HA	1:B:26:ILE:HB	1.84	0.59
1:A:79:ALA:O	1:A:83:LEU:HG	2.01	0.59
1:B:48:THR:HA	1:B:51:ILE:HD12	1.84	0.59
1:B:54:GLN:HG2	1:B:94:PHE:CD2	2.37	0.59
1:A:54:GLN:HE21	1:A:94:PHE:HB3	1.69	0.58
1:B:84:GLU:HA	1:B:87:MET:HG3	1.86	0.58
1:B:290:ALA:HB2	1:B:314:PHE:HB3	1.86	0.58
1:A:23:PHE:HA	1:A:26:ILE:HB	1.85	0.58
1:B:54:GLN:HE21	1:B:94:PHE:HB3	1.69	0.58
1:B:89:GLU:O	1:B:93:LEU:HG	2.04	0.58
1:B:58:LEU:O	1:B:61:LEU:HG	2.04	0.58
1:A:89:GLU:O	1:A:93:LEU:HG	2.04	0.57
1:A:58:LEU:O	1:A:61:LEU:HG	2.04	0.57
1:A:112:VAL:HG12	1:A:113:LEU:HD23	1.84	0.57
1:A:84:GLU:HA	1:A:87:MET:HG3	1.85	0.57
1:A:290:ALA:HB2	1:A:314:PHE:HB3	1.86	0.56
1:A:161:ASP:O	1:A:165:ASN:ND2	2.39	0.56
1:B:66:LYS:O	1:B:69:LYS:HG2	2.05	0.56
1:B:161:ASP:O	1:B:165:ASN:ND2	2.39	0.56
1:B:35:LEU:O	1:B:38:GLU:HG2	2.07	0.55
1:B:158:ARG:NH2	1:B:210:TRP:O	2.39	0.55
1:A:66:LYS:O	1:A:69:LYS:HG2	2.05	0.55
1:A:35:LEU:O	1:A:38:GLU:HG2	2.07	0.55
1:A:158:ARG:NH2	1:A:210:TRP:O	2.40	0.55
1:B:37:LEU:HD12	1:B:37:LEU:O	2.06	0.55
1:A:48:THR:HA	1:A:51:ILE:CD1	2.36	0.54
1:B:219:PHE:CZ	1:B:293:LEU:HD22	2.44	0.53
1:A:219:PHE:CZ	1:A:293:LEU:HD22	2.44	0.52
1:B:56:LYS:HZ2	1:B:57:ARG:HG2	1.75	0.52
1:A:112:VAL:O	1:B:178:ARG:NE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TYR:HE2	1:B:44:GLN:HG3	1.75	0.52
1:B:25:ASN:O	1:B:29:THR:HG23	2.10	0.51
1:B:48:THR:HA	1:B:51:ILE:CD1	2.40	0.51
1:B:152:ARG:HG3	1:B:153:PHE:CD1	2.45	0.51
1:A:152:ARG:HG3	1:A:153:PHE:CD1	2.45	0.51
1:B:140:LEU:HD21	1:B:170:TRP:HZ3	1.76	0.51
1:B:54:GLN:O	1:B:58:LEU:HB2	2.11	0.51
1:B:78:GLY:O	1:B:82:GLU:HG2	2.11	0.51
1:A:44:GLN:O	1:A:48:THR:HG23	2.11	0.51
1:A:78:GLY:O	1:A:82:GLU:HG2	2.11	0.50
1:A:140:LEU:HD21	1:A:170:TRP:HZ3	1.76	0.50
1:B:140:LEU:HD23	1:B:171:TYR:HD2	1.77	0.50
1:A:25:ASN:O	1:A:29:THR:HG23	2.11	0.50
1:A:20:GLN:O	1:A:24:GLN:HG3	2.12	0.50
1:A:47:CYS:O	1:A:50:SER:HB3	2.11	0.50
1:A:37:LEU:HA	1:B:40:LEU:HD11	1.94	0.50
1:A:37:LEU:HD12	1:A:37:LEU:O	2.11	0.49
1:B:20:GLN:O	1:B:24:GLN:HG3	2.12	0.49
1:A:54:GLN:O	1:A:58:LEU:HB2	2.13	0.49
1:A:140:LEU:HD23	1:A:171:TYR:HD2	1.77	0.49
1:A:56:LYS:HZ2	1:A:57:ARG:HG2	1.78	0.49
1:B:83:LEU:O	1:B:86:GLN:NE2	2.46	0.48
1:A:83:LEU:O	1:A:86:GLN:NE2	2.46	0.48
1:B:242:SER:OG	1:B:243:GLY:N	2.47	0.48
1:A:19:LEU:HD12	1:A:22:ASP:HB2	1.96	0.48
1:A:242:SER:OG	1:A:243:GLY:N	2.47	0.48
1:B:51:ILE:O	1:B:55:LYS:HG2	2.14	0.48
1:A:68:CYS:SG	1:A:80:ALA:HB2	2.54	0.47
1:B:19:LEU:HD12	1:B:22:ASP:HB2	1.96	0.47
1:B:68:CYS:SG	1:B:80:ALA:HB2	2.54	0.47
1:A:51:ILE:O	1:A:55:LYS:HG2	2.14	0.47
1:A:81:GLN:HA	1:A:81:GLN:OE1	2.15	0.47
1:A:48:THR:HA	1:A:51:ILE:HD12	1.96	0.47
1:B:39:GLU:HA	1:B:42:LYS:NZ	2.30	0.47
1:A:39:GLU:HA	1:A:42:LYS:NZ	2.30	0.46
1:B:81:GLN:HA	1:B:81:GLN:OE1	2.15	0.46
1:B:102:PRO:HG3	1:B:121:LEU:HD23	1.98	0.46
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.76	0.45
1:A:90:ARG:HH21	1:B:19:LEU:HG	1.81	0.45
1:A:48:THR:HA	1:A:51:ILE:HG13	1.97	0.45
1:A:103:LYS:NZ	1:A:184:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.82	0.44
1:A:120:LEU:HB2	1:A:185:ASN:HD21	1.83	0.44
1:A:326:LEU:HD13	1:A:326:LEU:HA	1.87	0.44
1:B:48:THR:O	1:B:52:THR:HG23	2.18	0.44
1:A:84:GLU:HA	1:A:87:MET:CG	2.47	0.44
1:A:39:GLU:HG2	1:A:42:LYS:HZ3	1.83	0.44
1:A:11:ASP:N	1:A:11:ASP:OD1	2.51	0.43
1:B:39:GLU:HG2	1:B:42:LYS:HZ3	1.83	0.43
1:B:120:LEU:HB2	1:B:185:ASN:HD21	1.83	0.43
1:B:302:CYS:SG	1:B:303:LYS:N	2.86	0.43
1:A:210:TRP:HA	1:A:306:GLN:OE1	2.19	0.43
1:B:11:ASP:N	1:B:11:ASP:OD1	2.51	0.43
1:B:195:PHE:HA	1:B:198:TYR:HB2	2.01	0.43
1:B:317:LEU:HA	1:B:317:LEU:HD23	1.82	0.43
1:A:40:LEU:HA	1:A:40:LEU:HD23	1.76	0.43
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.82	0.43
1:B:210:TRP:HA	1:B:306:GLN:OE1	2.19	0.43
1:A:40:LEU:HD11	1:B:37:LEU:HA	2.01	0.42
1:A:109:LEU:HD12	1:A:109:LEU:HA	1.76	0.42
1:B:103:LYS:NZ	1:B:184:ASN:OD1	2.49	0.42
1:A:222:GLN:HB3	1:A:289:ASN:OD1	2.20	0.42
1:B:326:LEU:HA	1:B:329:VAL:HG12	2.02	0.42
1:A:178:ARG:NE	1:B:112:VAL:O	2.49	0.42
1:A:195:PHE:HA	1:A:198:TYR:HB2	2.01	0.42
1:A:326:LEU:HA	1:A:329:VAL:HG12	2.02	0.42
1:B:276:LEU:N	1:B:277:PRO:HD2	2.35	0.42
1:A:102:PRO:HG3	1:A:121:LEU:HD23	2.02	0.41
1:A:302:CYS:SG	1:A:303:LYS:N	2.86	0.41
1:B:84:GLU:HA	1:B:87:MET:CG	2.47	0.41
1:A:276:LEU:N	1:A:277:PRO:HD2	2.35	0.41
1:B:222:GLN:HB3	1:B:289:ASN:OD1	2.20	0.41
1:B:158:ARG:HH21	1:B:210:TRP:HB2	1.86	0.41
1:A:56:LYS:HB3	1:A:56:LYS:HE3	1.88	0.41
1:A:57:ARG:HD3	1:A:57:ARG:HA	1.92	0.41
1:A:307:VAL:HG23	1:A:308:LEU:N	2.36	0.41
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.82	0.41
1:B:57:ARG:HA	1:B:57:ARG:HD3	1.92	0.41
1:A:312:PHE:O	1:A:313:PRO:C	2.60	0.41
1:A:226:PHE:HD1	1:A:285:TRP:HD1	1.69	0.40
1:B:8:PRO:HB2	1:B:9:LEU:H	1.59	0.40
1:A:158:ARG:HH21	1:A:210:TRP:HB2	1.85	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	303/625 (48%)	281 (93%)	21 (7%)	1 (0%)	41	72
1	B	303/625 (48%)	283 (93%)	19 (6%)	1 (0%)	41	72
All	All	606/1250 (48%)	564 (93%)	40 (7%)	2 (0%)	44	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	ASP
1	B	299	ASP

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	280/552 (51%)	269 (96%)	11 (4%)	32	61
1	B	280/552 (51%)	271 (97%)	9 (3%)	39	67
All	All	560/1104 (51%)	540 (96%)	20 (4%)	38	63

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU

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Mol	Chain	Res	Type
1	A	37	LEU
1	A	47	CYS
1	A	75	GLU
1	A	84	GLU
1	A	88	LYS
1	A	121	LEU
1	A	132	GLU
1	A	242	SER
1	A	286	GLN
1	A	313	PRO
1	B	9	LEU
1	B	37	LEU
1	B	47	CYS
1	B	75	GLU
1	B	84	GLU
1	B	88	LYS
1	B	132	GLU
1	B	242	SER
1	B	286	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	54	GLN
1	A	165	ASN
1	A	185	ASN
1	A	336	GLN
1	B	44	GLN
1	B	54	GLN
1	B	165	ASN
1	B	185	ASN
1	B	336	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 monosaccharides 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.

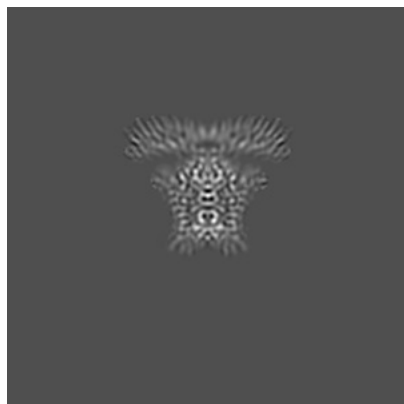
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30495. These allow visual inspection of the internal detail of the map and identification of artifacts.

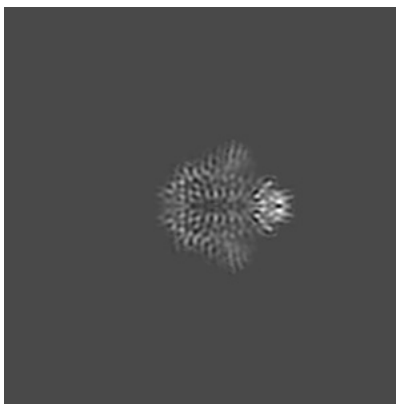
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

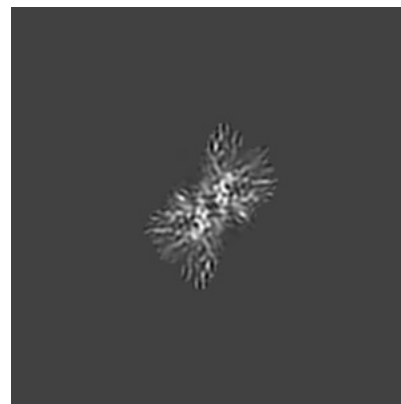
6.1.1 Primary map



X

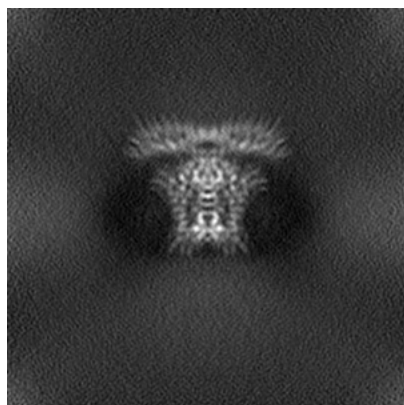


Y

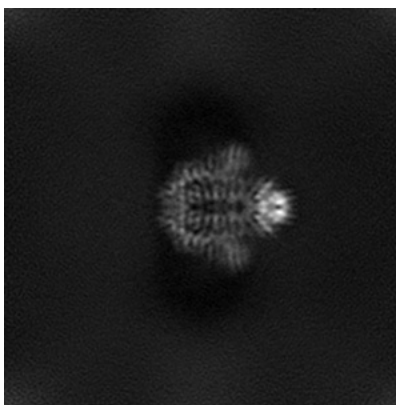


Z

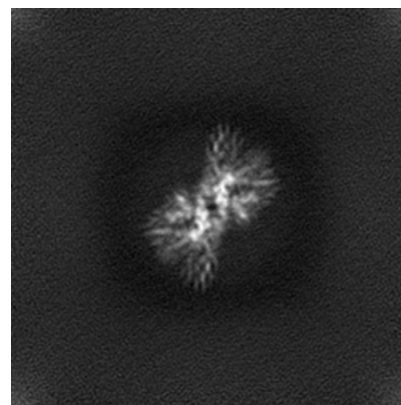
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

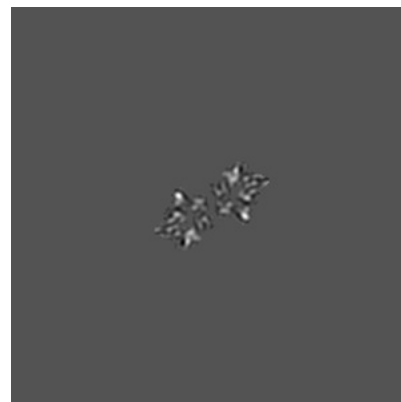
6.2.1 Primary map



X Index: 110

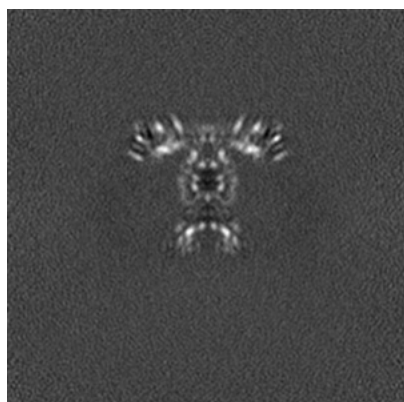


Y Index: 110

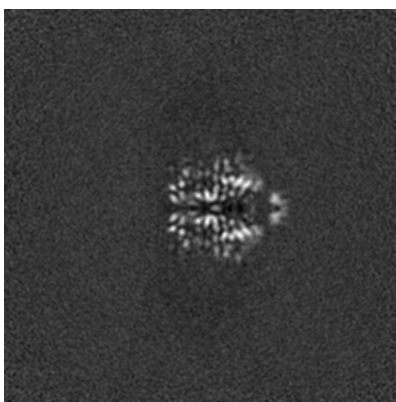


Z Index: 110

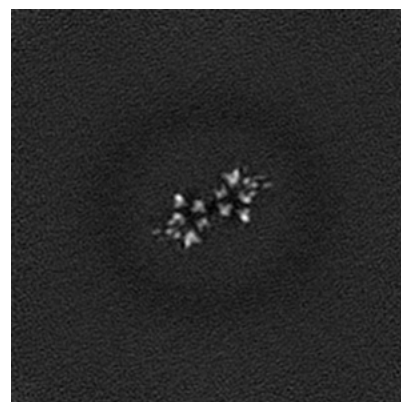
6.2.2 Raw map



X Index: 110



Y Index: 110



Z Index: 110

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: 105

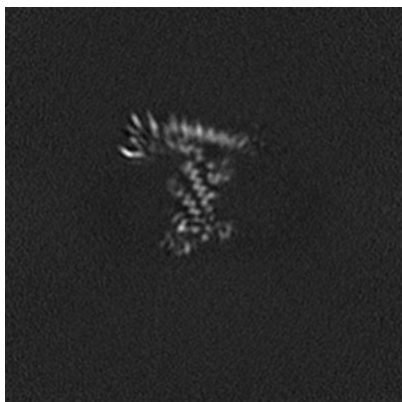


Y Index: 106

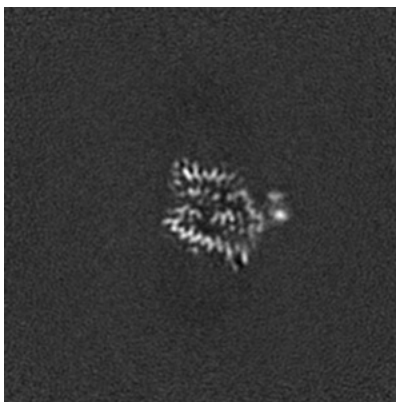


Z Index: 98

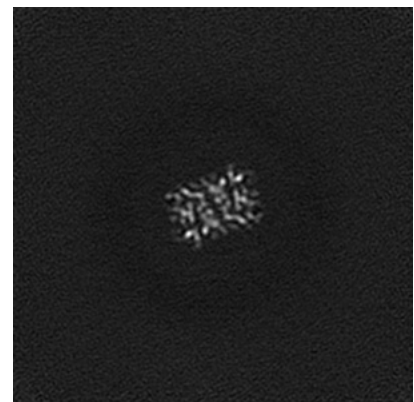
6.3.2 Raw map



X Index: 105



Y Index: 106

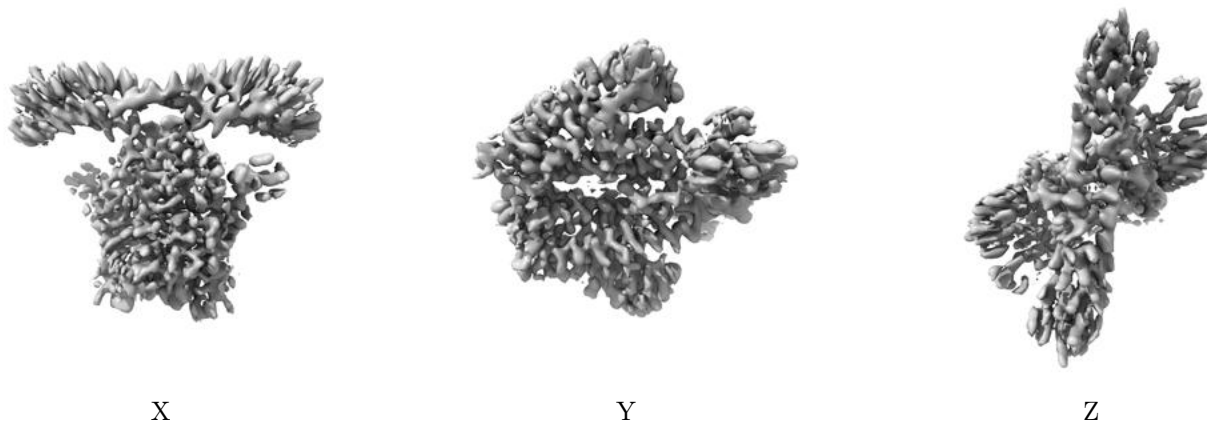


Z Index: 98

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

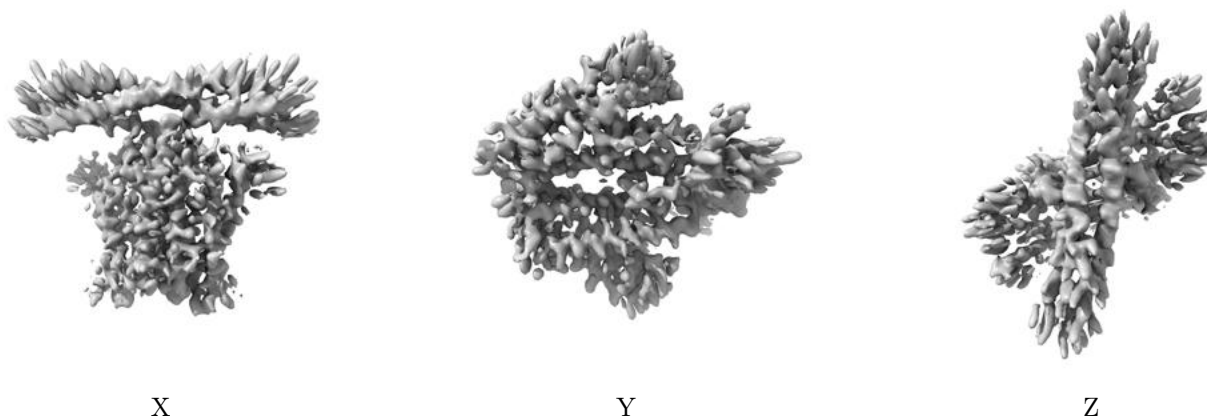
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

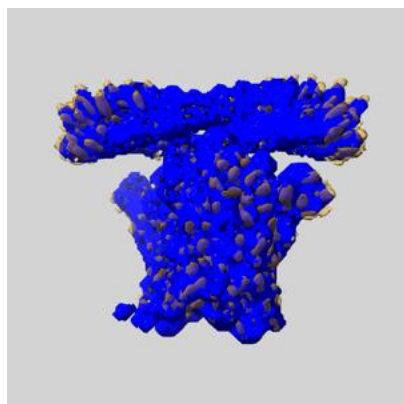
6.5 Mask visualisation [i](#)

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

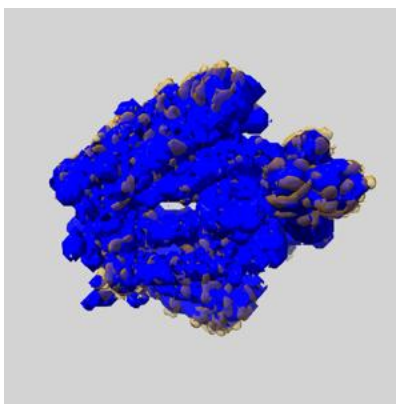
A mask typically either:

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

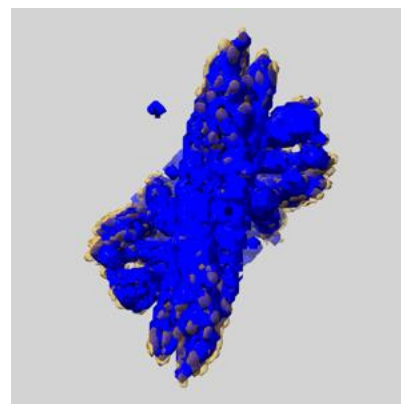
6.5.1 emd_30495_msk_1.map [i](#)



X



Y

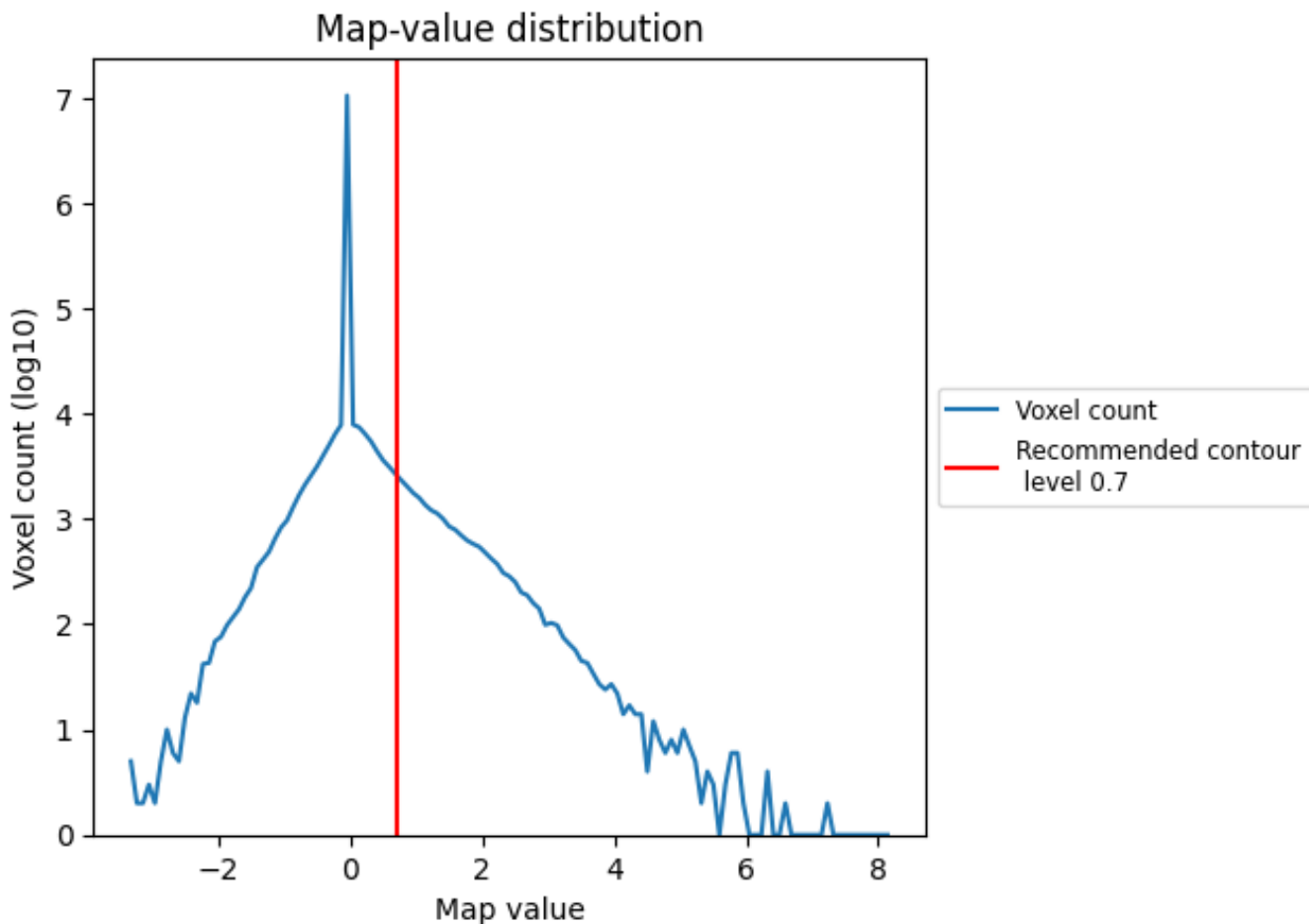


Z

7 Map analysis [i](#)

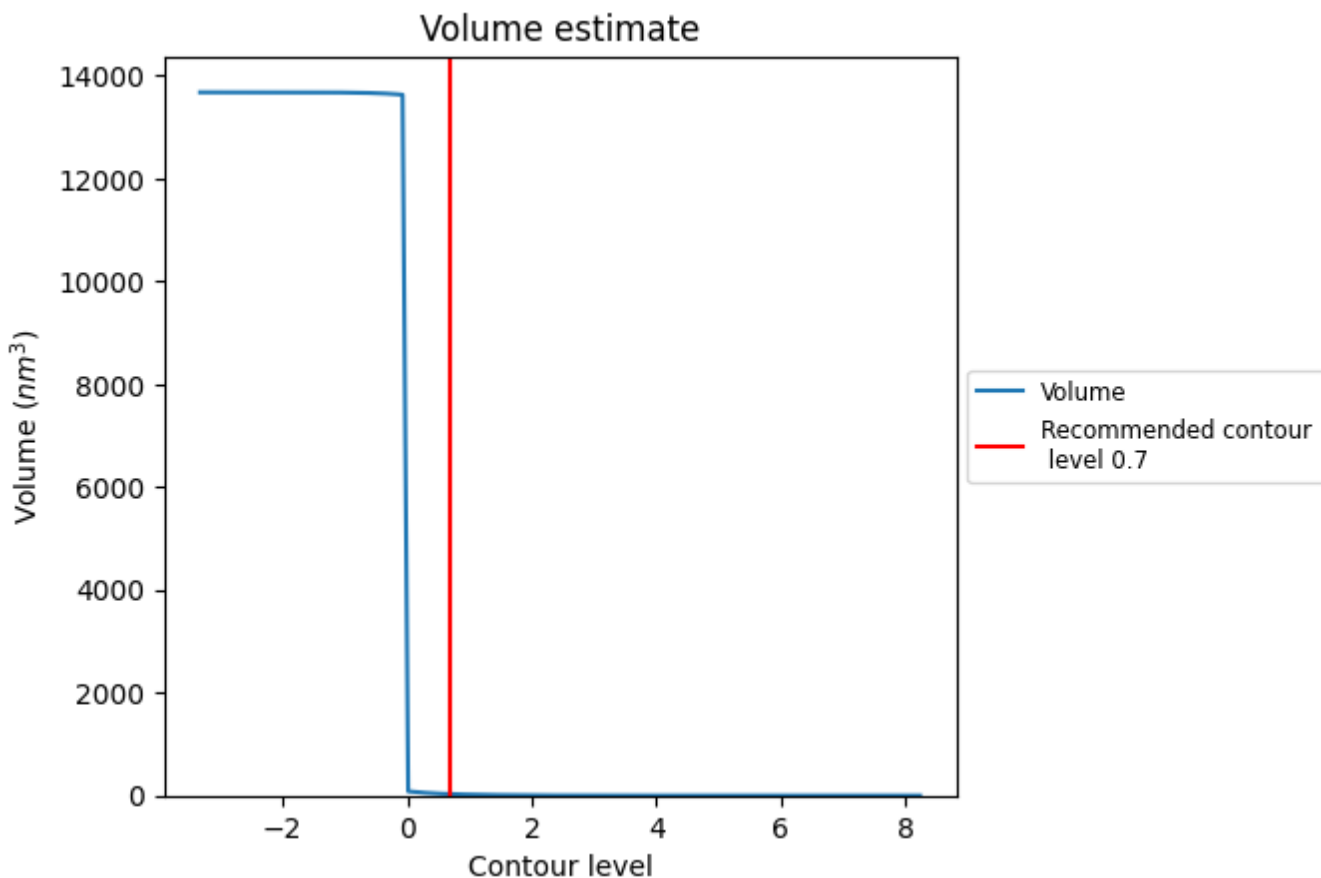
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

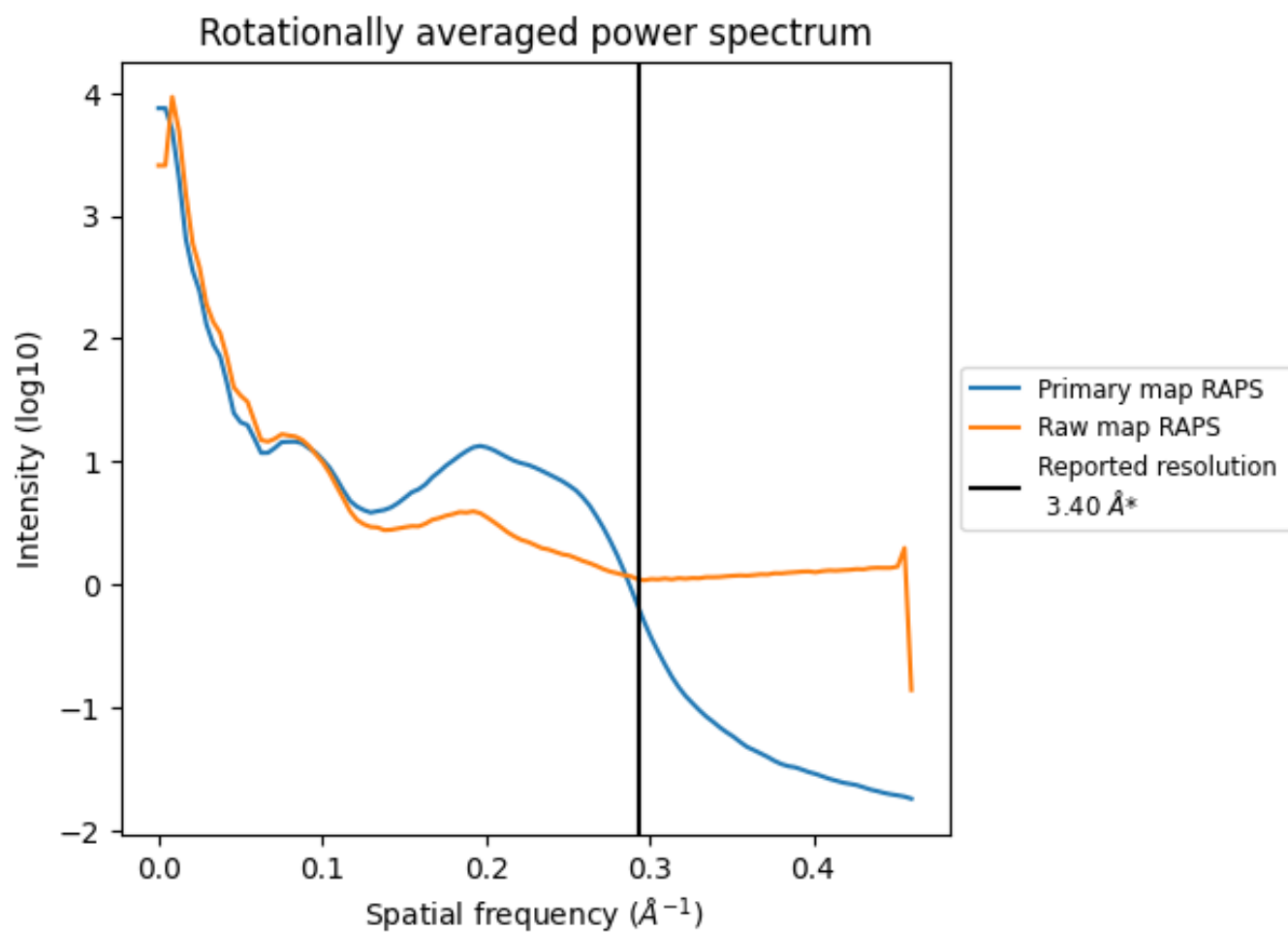
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 29 nm³; this corresponds to an approximate mass of 26 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

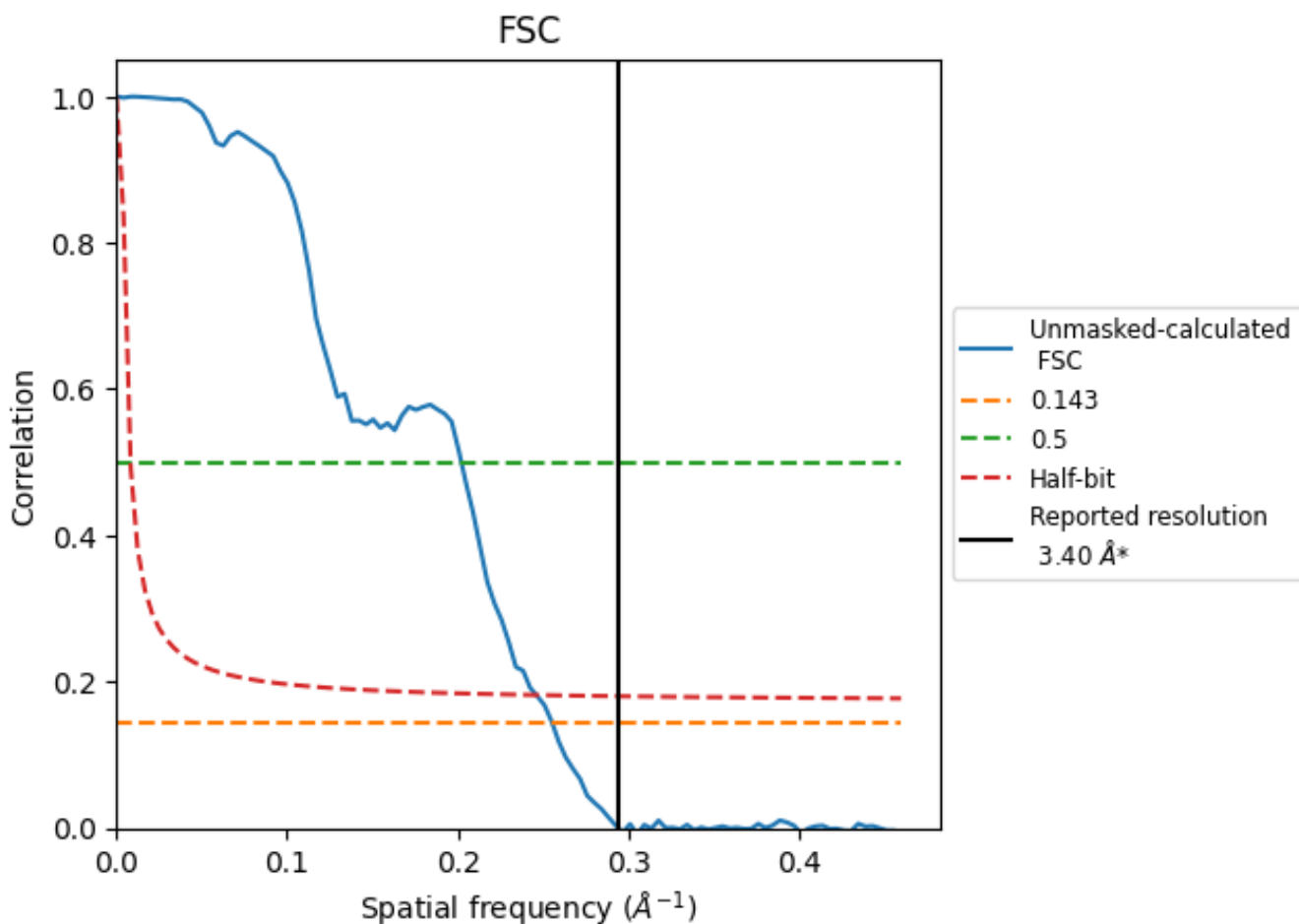


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

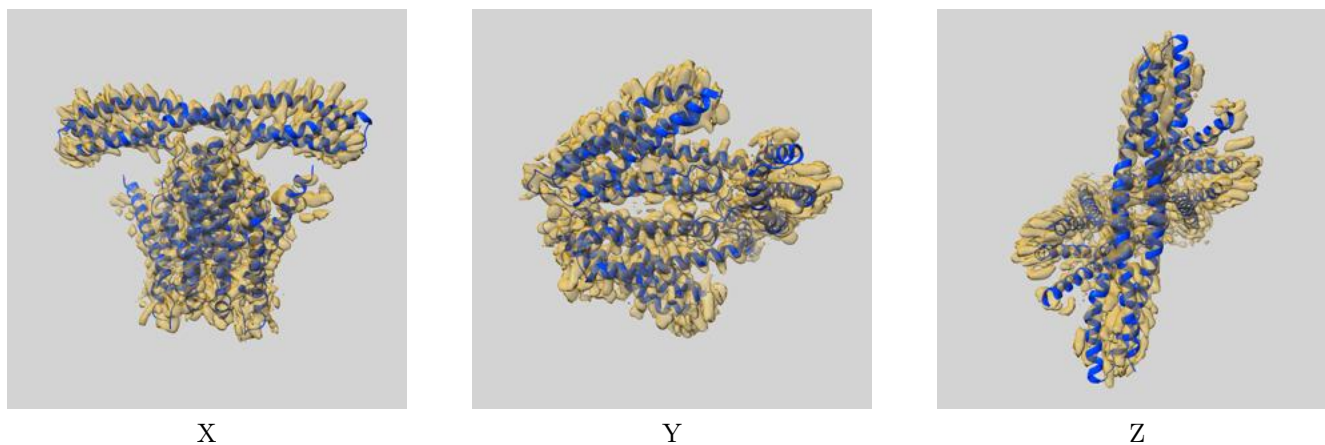
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	4.95	4.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

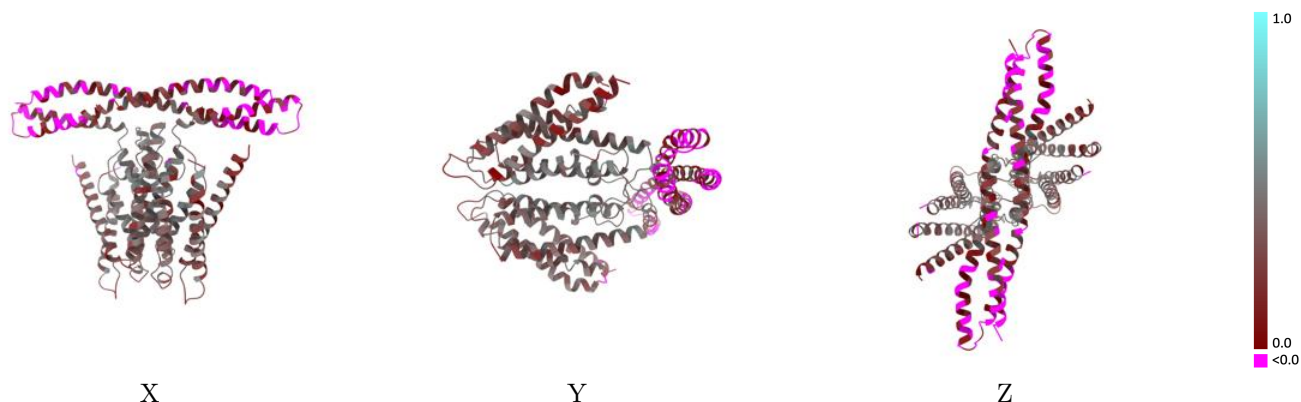
This section contains information regarding the fit between EMDB map EMD-30495 and PDB model 7CXR. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



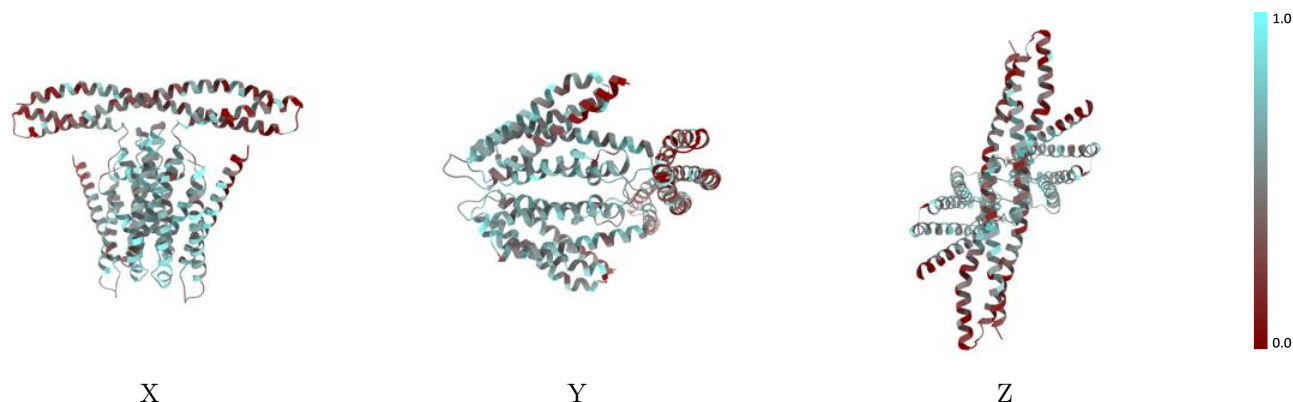
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



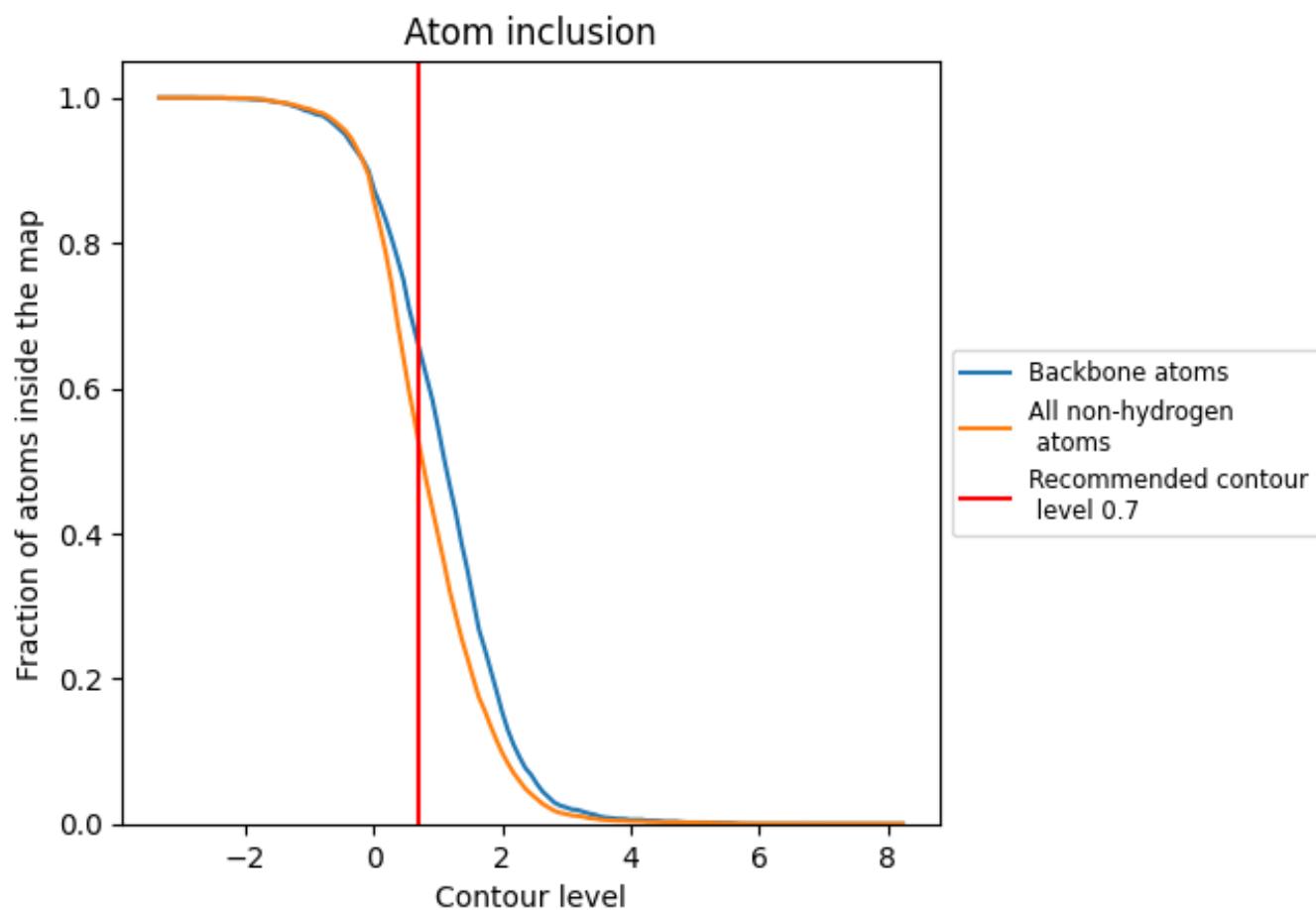
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	█ 0.5280	█ 0.2780
A	█ 0.5241	█ 0.2750
B	█ 0.5320	█ 0.2820

