



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 05:49 PM UTC

PDB ID : 5SV9 / pdb_00005sv9
EMDB ID : EMD-8313
Title : Structure of the SLC4 transporter Bor1p in an inward-facing conformation
Authors : Coudray, N.; Seyler, S.; Lasala, R.; Zhang, Z.; Clark, K.M.; Dumont, M.E.; Rohou, A.; Beckstein, O.; Stokes, D.L.; Transcontinental EM Initiative for Membrane Protein Structure (TEMIMPS)
Deposited on : 2016-08-05
Resolution : 5.90 Å (reported)
Based on initial model : 4YZF

This is a wwPDB EM Validation Summary 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

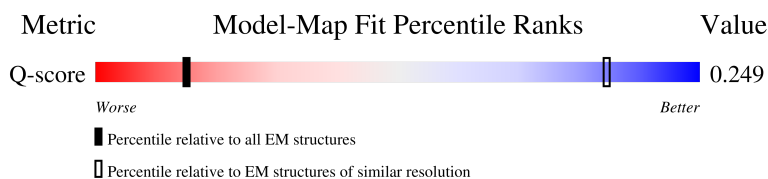
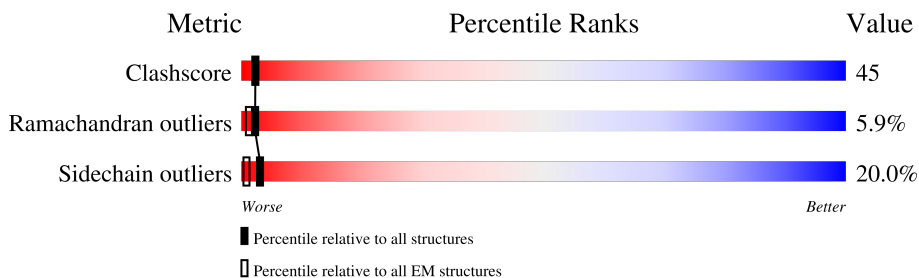
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.90 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	501 (5.40 - 6.40)

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	476	
1	B	476	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7612 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.

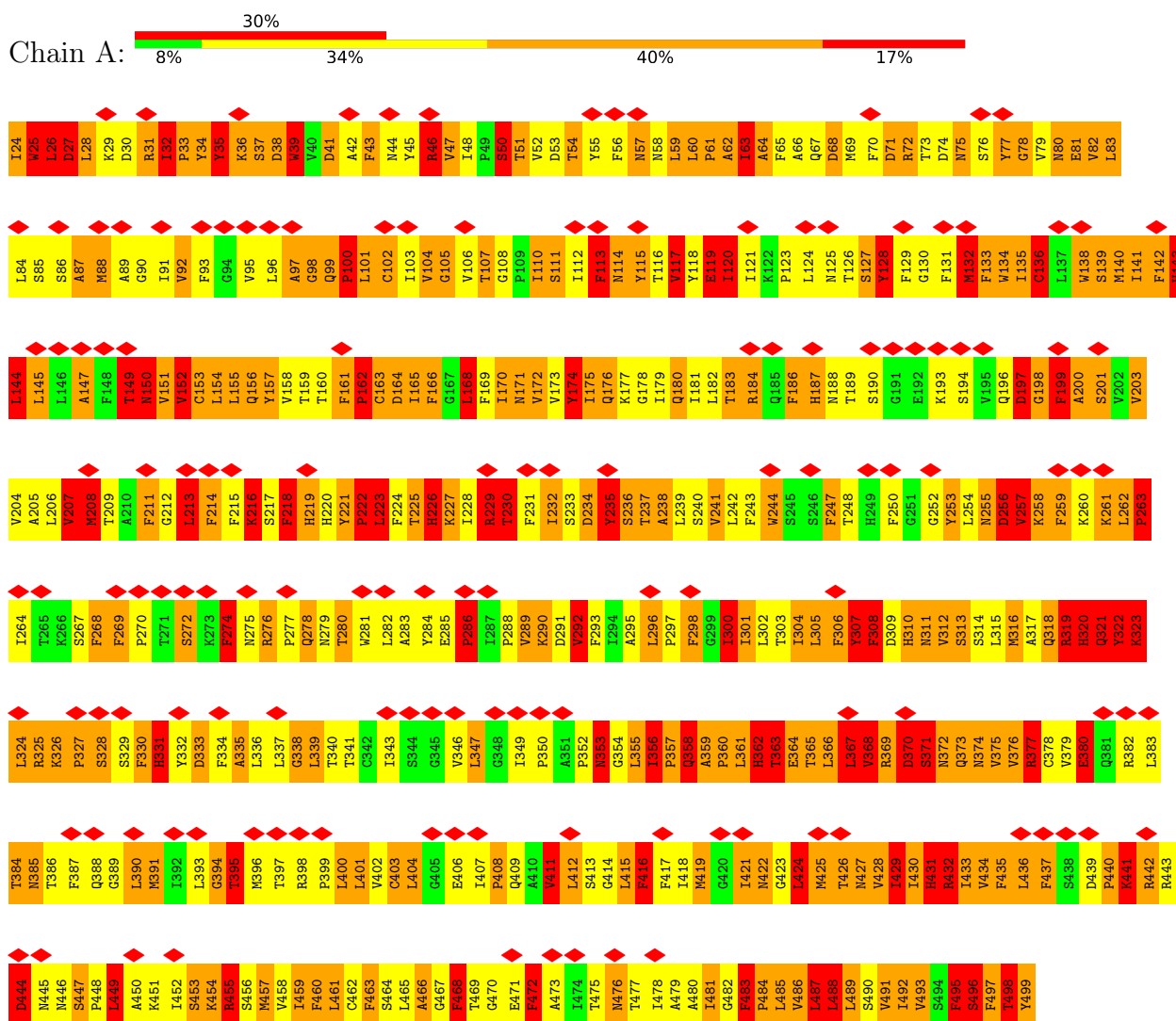
- Molecule 1 is a protein called Bor1p boron transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	476	Total	C	N	O	S	0	0
			3806	2527	608	652	19		
1	B	476	Total	C	N	O	S	0	0
			3806	2527	608	652	19		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Bor1p boron transporter



• Molecule 1: Bor1p boron transporter



P448	G388	S328	K266	L206	L145	L84	T24
L449	G389	S329	S267	V207	L146	S85	K25
A450	L390	F330	F268	M208	A147	A87	L26
K451	M391	H331	F269	T209	F148	M88	D27
I452	I392	H332	K273	A210	T149		L28
S453	D383	D383	F274	F211	N150		K29
K454	G394	F334	M275	G212	I91		D30
R455	T395	A335	F276	L213	V92		R31
S456	K396	A336	R276	L214	V92		I32
M457	T397	L336	P277	F215	C153		F33
R398	L337	L337	Q278	K216	F93		F34
V458	G338	L339	N279	S217	G94		Y35
I459	P399	L339	T280	F218	V95		K36
F460	L400	T340	V281		L96		S37
L461	L401	T341	L282	H219	V158		D38
F463	V402	C342	A283	H220	T159		K39
S464	C403	I343	Y284	Y221	T160		V40
L465	L404	S344	E285	P222	F161		D41
A466	G405	G345	P286	L223	P162		A42
G467	E406	V346	T287	T224	C163		F43
F468	P408	L347	P288	T225	D164		N44
T469	I407	L347	T289	H226	T165		Y45
G470	Q409	G348	K290	K227	F166		N46
E471	A410	I349	D291	I228	G105		R46
F472	V411	P350	V292	R229	V106		V47
A473	L412	A351	F293	T230	I170		I48
I474	P352	P352	T294	F231	G108		F49
T475	S413	N353	A295	I232	P109		S50
L476	G414	G354	L296	S233	I110		T51
N477	L415	L355	P297	I175	S111		V52
F478	F416	L356	F298	D234	I112		D53
A479	F417	P357	C299	Y235	Q176		T54
M419	I418	Q358	I300	S236	M113		Y55
G420	M419	Q358	T237	T237	Y115		F56
G421	A359	A359	I301	A238	T116		N57
I421	P360	P360	L302	L239	V117		N58
N422	L361	T361	T303	S240	Y118		L59
G423	H362	T363	F304	L182	E119		L60
L424	E364	E364	L305	T183	P61		P61
M425	T365	T365	F306	R184	A62		A62
T426	L366	L367	Y307	Q185	K122		A64
M427	L367	L367	F308	F186	P123		A64
V428	L368	V368	D309	H187	L124		F65
I429	R369	R369	H310	H188	N125		A66
I430	D370	D370	N311	T189	Q67		Q67
H431	S371	S371	V312	S127	D68		N69
R432	N372	N372	S313	Y128	F70		F70
I433	Q373	Q373	S314	G191	D71		D71
V434	N374	N374	L315	E192	G130		R72
F435	V375	V375	M316	K193	F131		T73
L436	V376	V376	A317	S194	M132		D74
F437	R377	R377	Q318	V195	F133		N75
S438	R377	R377	R319	Q196	M134		S76
D439	C378	C378	H320	D197	I135		S77
P440	V379	V379	Q321	C198	Y77		G78
K441	E380	E380	Y322	G198	C136		G79
R442	Q381	Q381	K323	F199	L137		N80
R443	R382	R382	L324	A200	M138		E81
D444	L383	L383	R325	S201	S139		V82
N445	T384	T384	K326	V202	M140		L83
N446	N385	N385	P327	V203	I141		
S447	T386	T386	F387	V204	F142		
				I284	H143		
				T265	L144		

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=37.35°, rise=4.8 Å, axial sym=C1	Depositor
Number of segments used	75	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	850	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	19000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	478.502	Depositor
Minimum map value	-365.121	Depositor
Average map value	0.789	Depositor
Map value standard deviation	24.341	Depositor
Recommended contour level	130	Depositor
Map size (Å)	183.82, 183.82, 183.82	wwPDB
Map dimensions	101, 101, 101	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.82, 1.82, 1.82	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	3.18	497/3917 (12.7%)	2.83	420/5333 (7.9%)
1	B	3.07	485/3917 (12.4%)	2.76	404/5333 (7.6%)
All	All	3.12	982/7834 (12.5%)	2.79	824/10666 (7.7%)

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	49
1	B	0	40
All	All	0	89

The worst 5 of 982 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308	PHE	CA-C	-14.25	1.34	1.52
1	B	48	ILE	CA-CB	-14.11	1.46	1.54
1	B	309	ASP	CA-C	-13.70	1.35	1.52
1	A	432	ARG	CD-NE	12.99	1.64	1.46
1	A	430	ILE	CA-C	-12.79	1.36	1.52

The worst 5 of 824 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	ILE	N-CA-C	26.50	135.44	110.53
1	B	330	PHE	CA-CB-CG	22.69	136.49	113.80
1	B	289	VAL	N-CA-C	18.29	129.19	110.72
1	B	218	PHE	CA-CB-CG	-17.49	96.31	113.80
1	A	320	HIS	CA-CB-CG	15.83	129.63	113.80

There are no chirality outliers.

5 of 89 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	ARG	Sidechain
1	A	35	TYR	Sidechain
1	A	37	SER	Peptide,Mainchain
1	A	43	PHE	Sidechain
1	A	46	ARG	Mainchain

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	3806	0	3851	333	0
1	B	3806	0	3851	366	0
All	All	7612	0	7702	693	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 45.

The worst 5 of 693 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:107:THR:HG23	1:B:110:ILE:H	1.40	0.87
1:B:331:HIS:HE1	1:B:335:ALA:HB2	1.40	0.86
1:A:184:ARG:HA	1:A:187:HIS:CD2	2.12	0.84
1:A:39:TRP:H	1:A:39:TRP:CD1	1.93	0.82
1:B:143:HIS:CE1	1:B:338:GLY:HA3	2.16	0.79

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	474/476 (100%)	408 (86%)	45 (10%)	21 (4%)	2	17
1	B	474/476 (100%)	392 (83%)	47 (10%)	35 (7%)	1	10
All	All	948/952 (100%)	800 (84%)	92 (10%)	56 (6%)	2	13

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	ALA
1	A	100	PRO
1	A	102	CYS
1	A	106	VAL
1	A	190	SER

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	424/424 (100%)	350 (82%)	74 (18%)	2	9
1	B	424/424 (100%)	328 (77%)	96 (23%)	1	6
All	All	848/848 (100%)	678 (80%)	170 (20%)	3	7

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	256	ASP
1	B	391	MET
1	B	284	TYR
1	B	333	ASP
1	B	422	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	187	HIS
1	B	219	HIS
1	B	381	GLN
1	B	310	HIS
1	B	331	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-8313. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

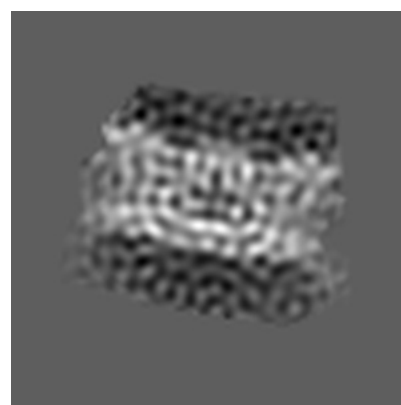
6.1.1 Primary map



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: 50



Y Index: 50



Z Index: 50

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: 39



Y Index: 46

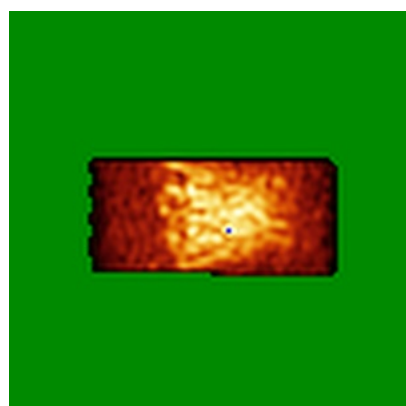


Z Index: 50

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

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

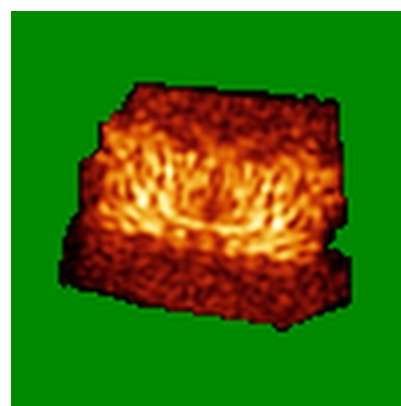
6.4.1 Primary map



X



Y

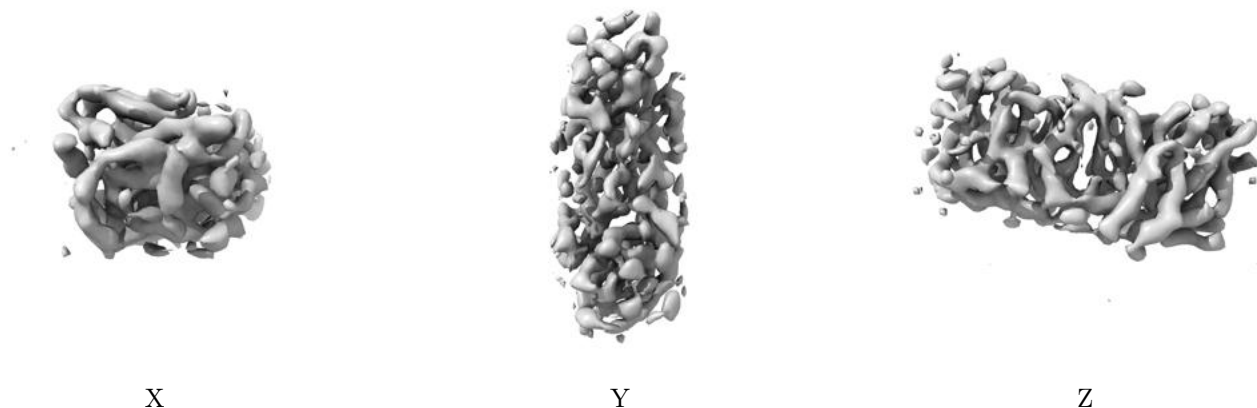


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 130.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

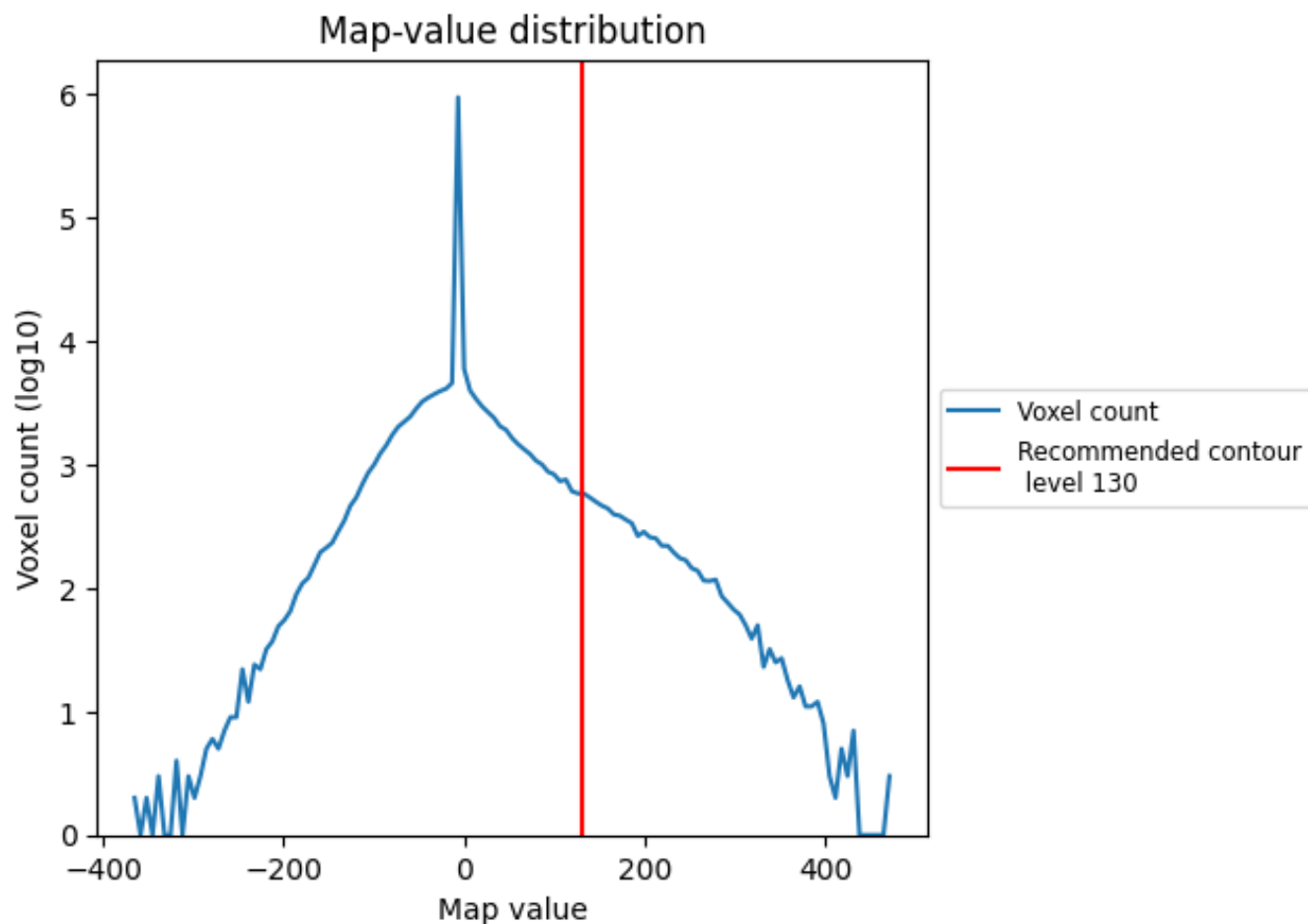
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

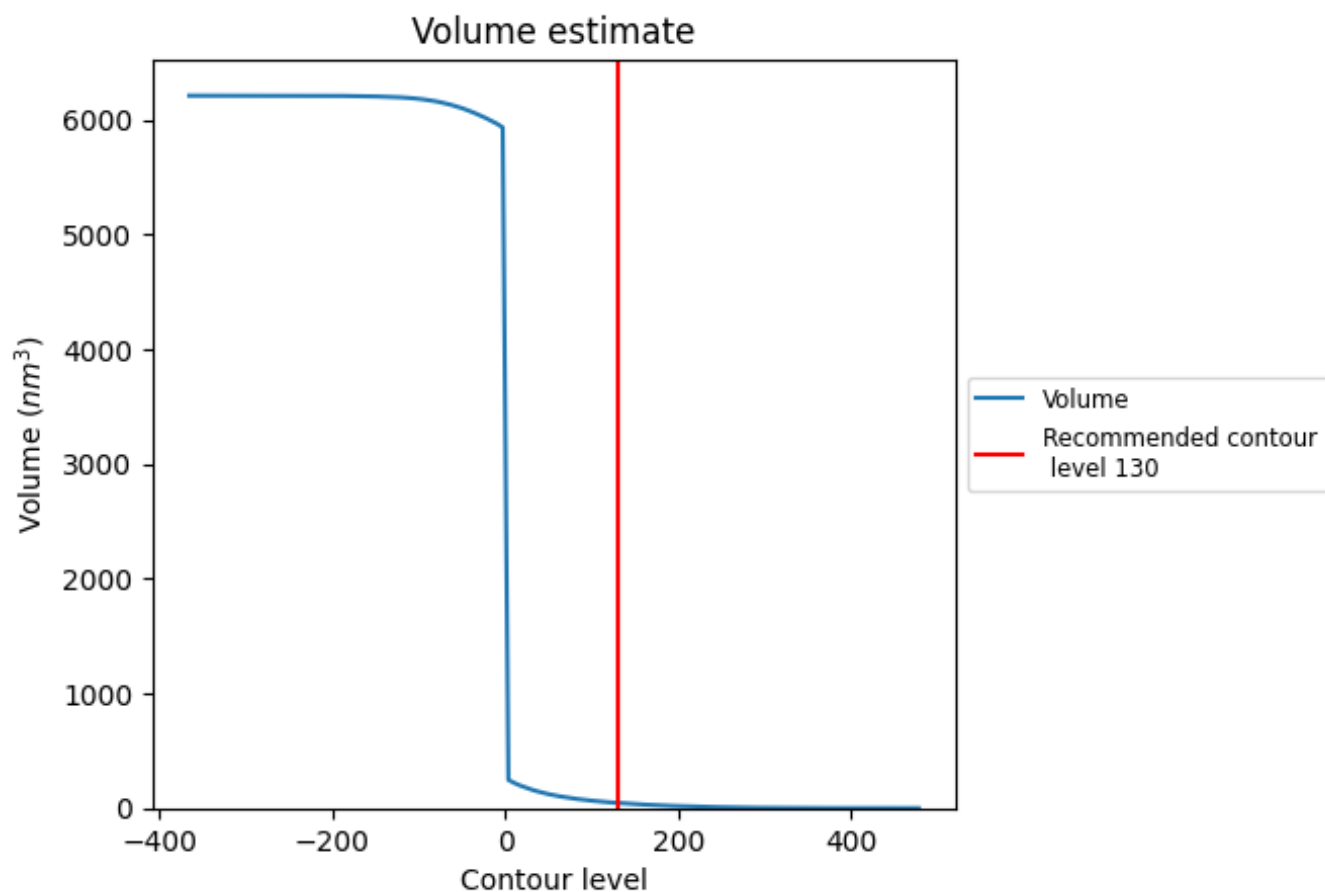
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

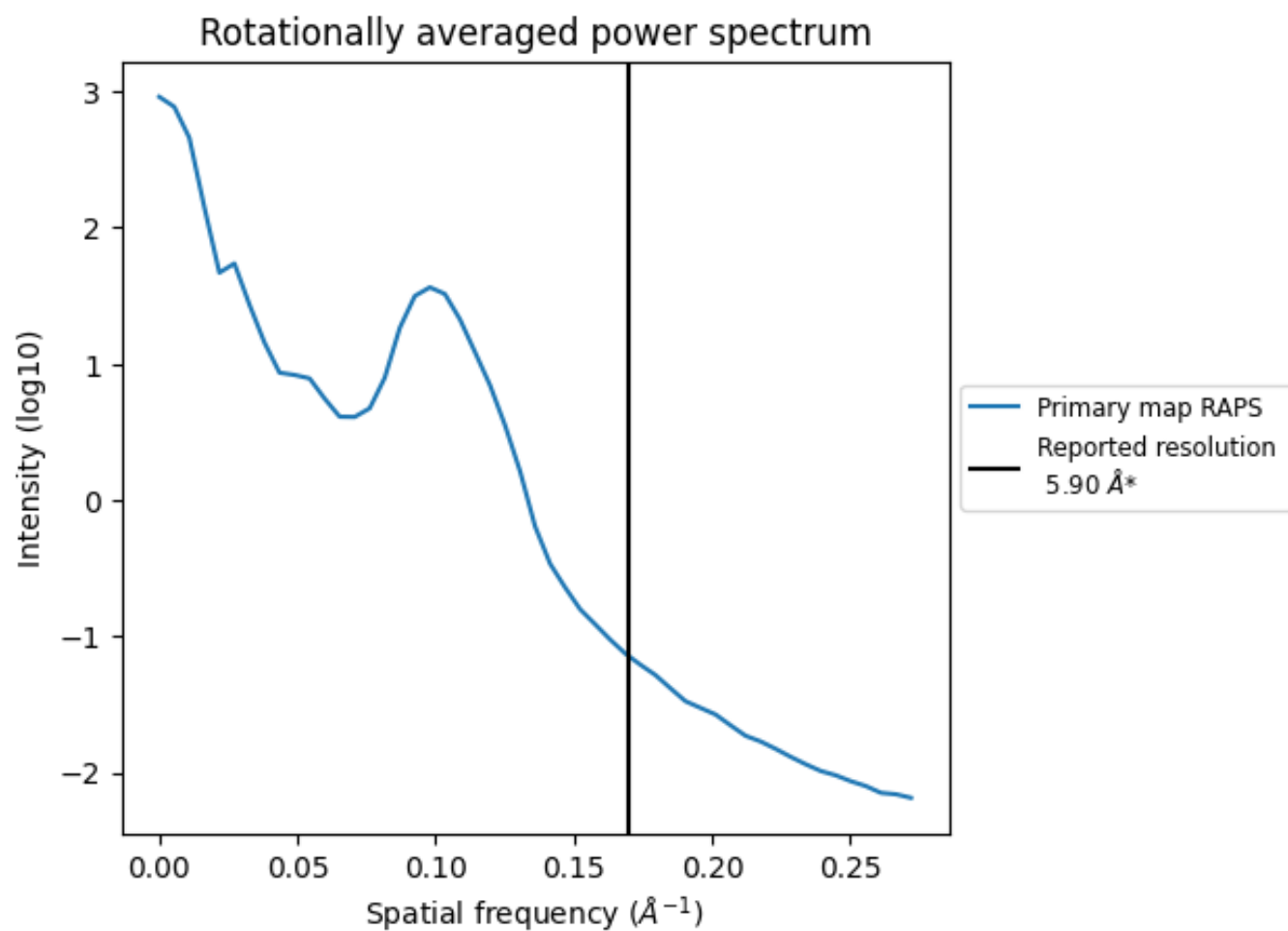
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm³; this corresponds to an approximate mass of 41 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 ⓘ

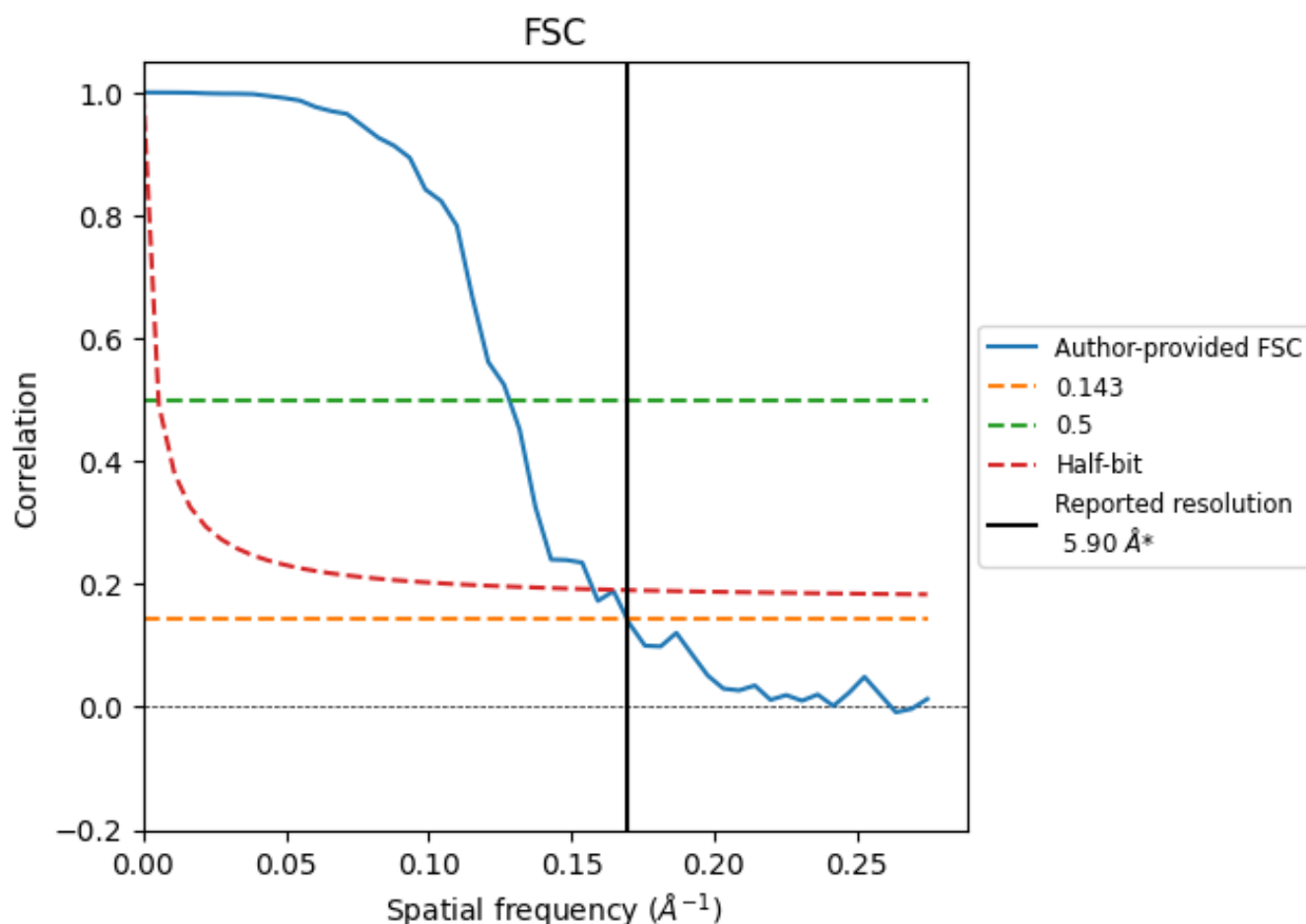


*Reported resolution corresponds to spatial frequency of 0.169 Å⁻¹

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 0.169 Å⁻¹

8.2 Resolution estimates [i](#)

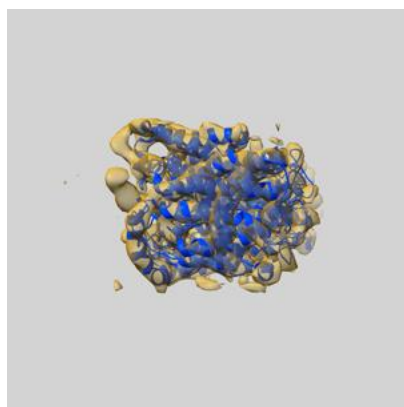
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.90	-	-
Author-provided FSC curve	5.90	7.80	6.34
Unmasked-calculated*	-	-	-

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

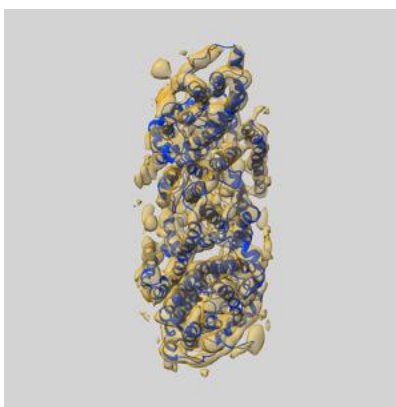
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8313 and PDB model 5SV9. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

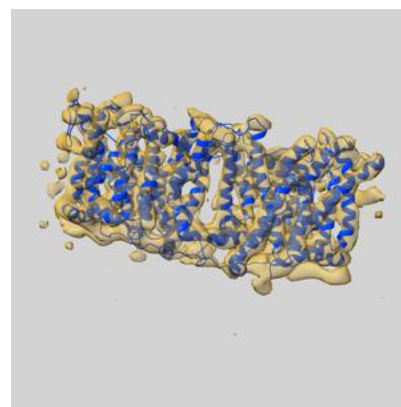
9.1 Map-model overlay [i](#)



X



Y



Z

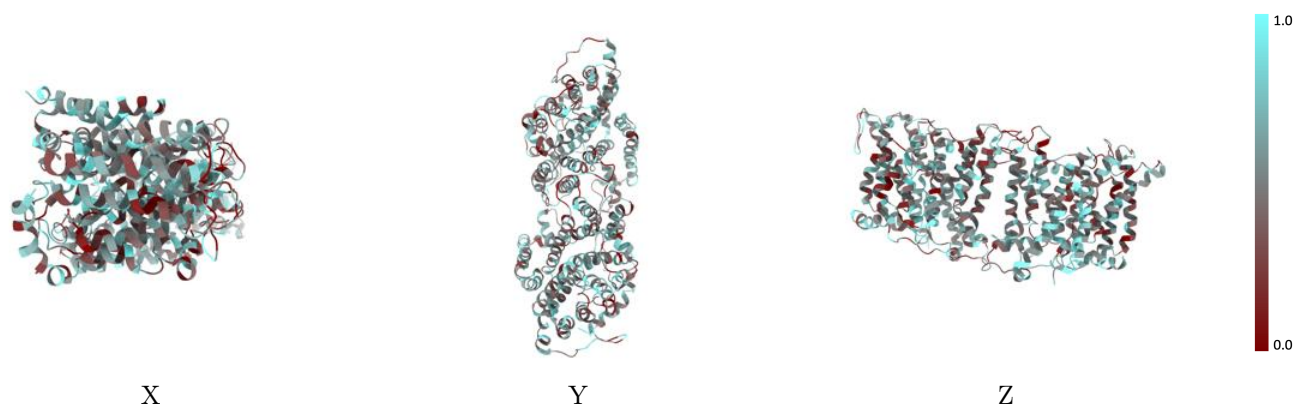
The images above show the 3D surface view of the map at the recommended contour level 130.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



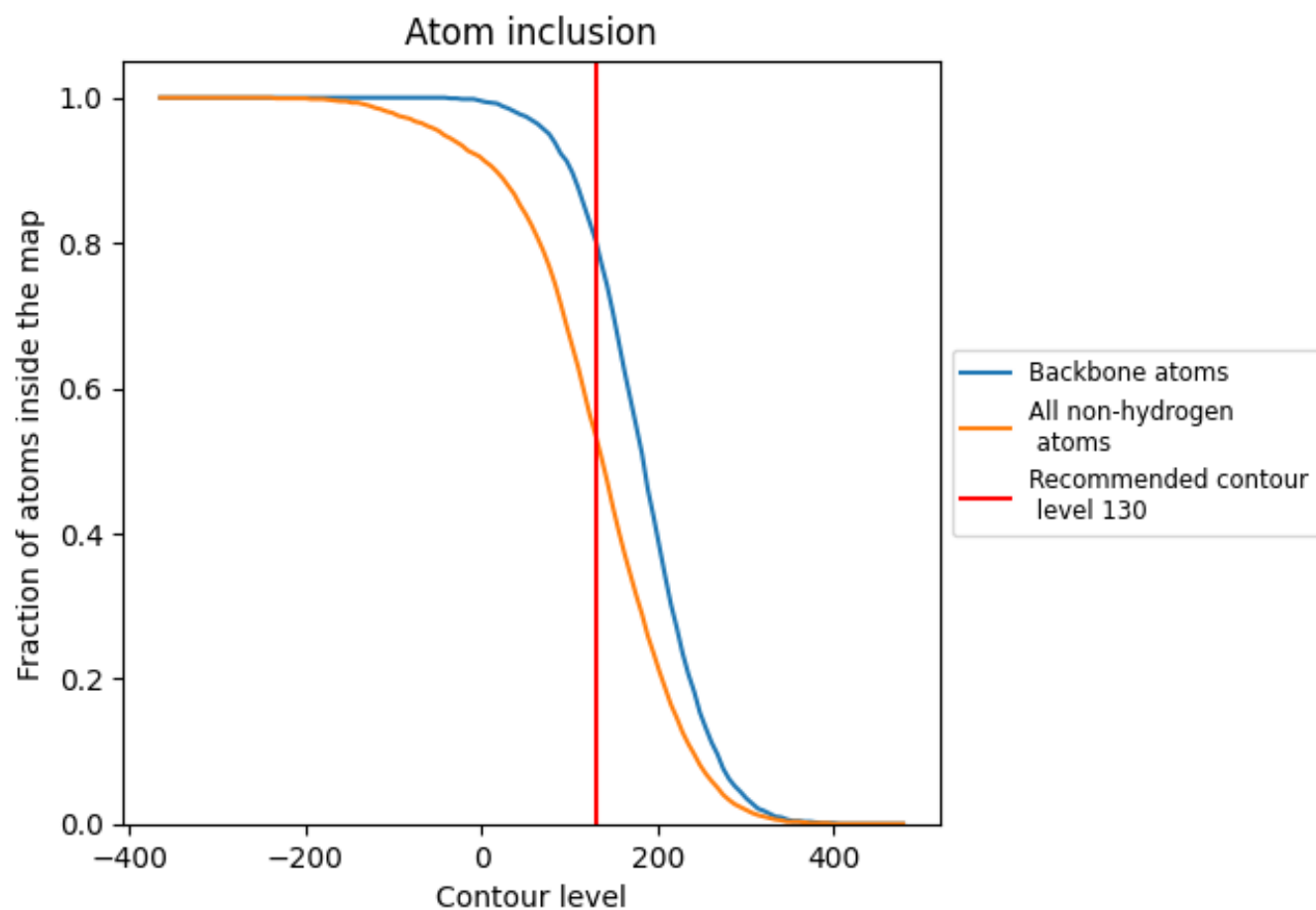
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (130).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 53% 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 (130) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5320	0.2490
A	0.5260	0.2440
B	0.5370	0.2540

