



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2024 – 01:31 pm BST

PDB ID : 8ATO
EMDB ID : EMD-15654
Title : Structure of the giant inhibitor of apoptosis, BIRC6 bound to the regulator SMAC
Authors : Dietz, L.; Elliott, P.R.
Deposited on : 2022-08-23
Resolution : 3.00 Å(reported)

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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

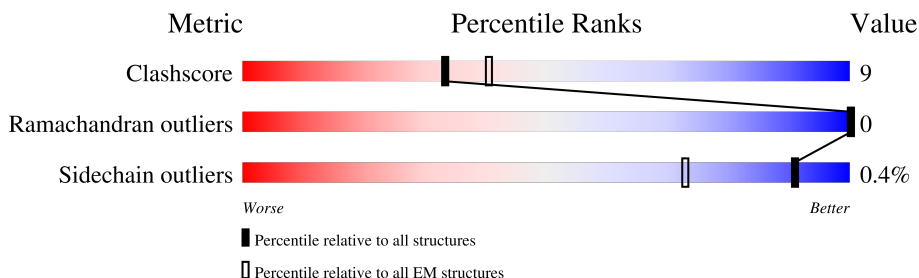
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	4859	<div> <div>20%</div> <div>47%</div> <div>12%</div> <div>41%</div> </div>
1	B	4859	<div> <div>17%</div> <div>45%</div> <div>14%</div> <div>40%</div> </div>
2	C	184	<div> <div>68%</div> <div>61%</div> <div>20%</div> <div>18%</div> </div>
2	D	184	<div> <div>71%</div> <div>70%</div> <div>11%</div> <div>18%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 46909 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 Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2871	Total	C	N	O	S	0	0
			22195	14154	3782	4102	157		
1	B	2892	Total	C	N	O	S	0	0
			22348	14249	3807	4135	157		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9NR09
A	0	PRO	-	expression tag	UNP Q9NR09
B	-1	GLY	-	expression tag	UNP Q9NR09
B	0	PRO	-	expression tag	UNP Q9NR09

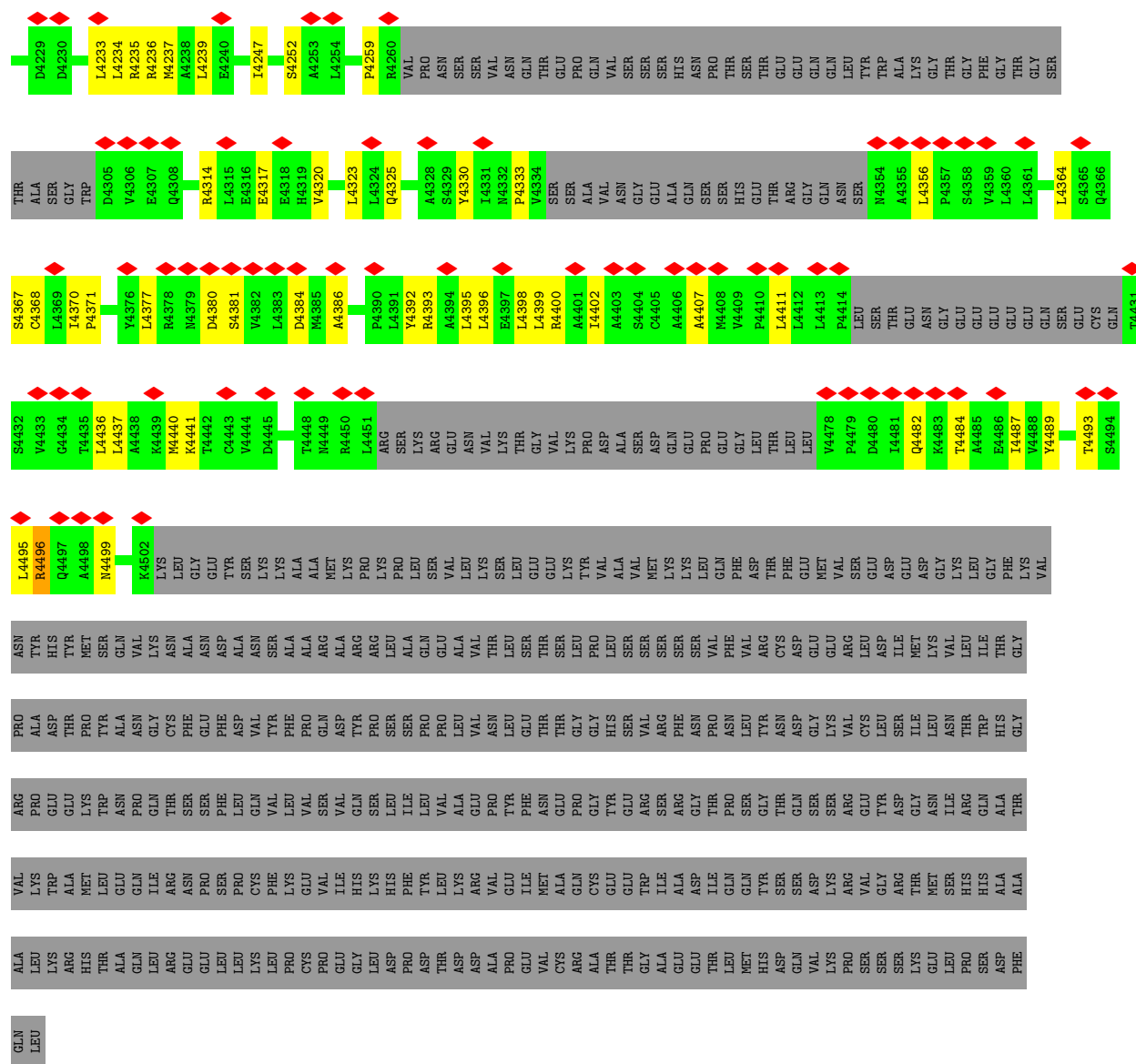
- Molecule 2 is a protein called Diablo IAP-binding mitochondrial protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	150	Total	C	N	O	S	0	0
			1183	739	198	241	5		
2	D	150	Total	C	N	O	S	0	0
			1183	739	198	241	5		

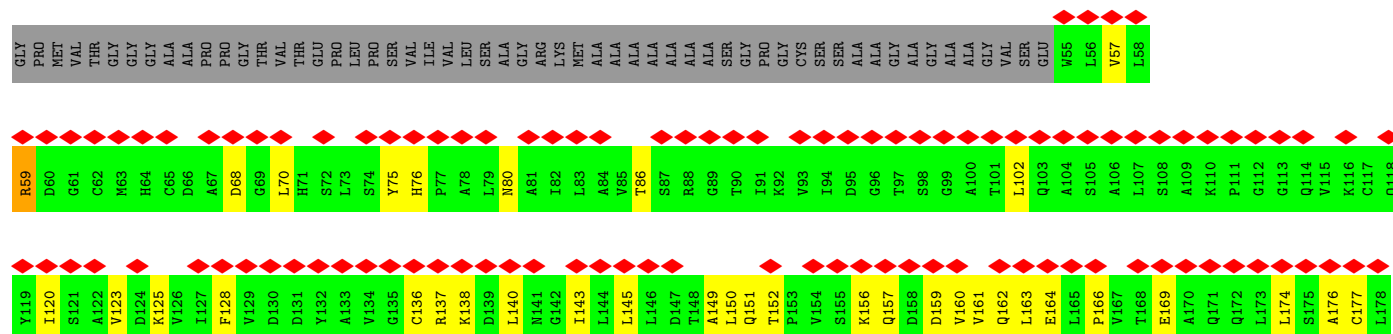








● Molecule 1: Baculoviral IAP repeat-containing protein 6





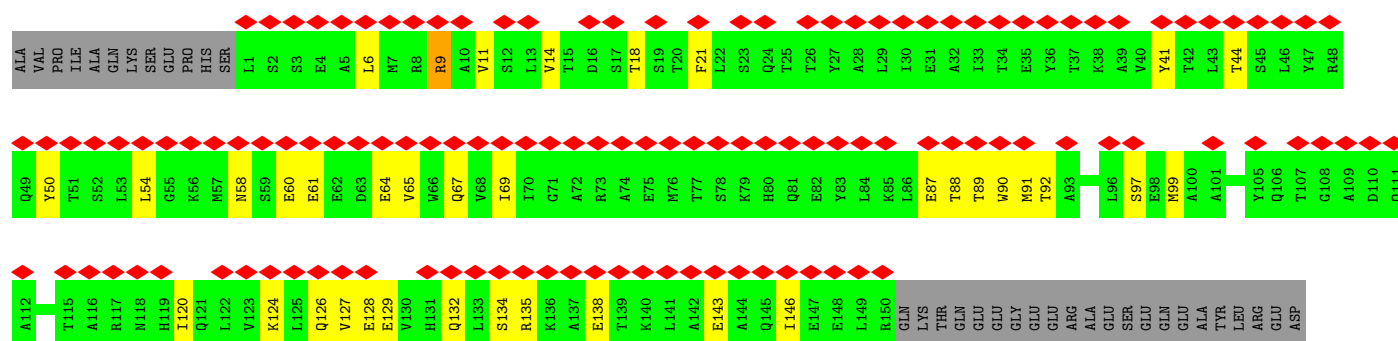


H3697	L3631	K3640	L3396	ARG	THR	L2923	L2813	GLU	K2597	PRO	SER	L2383	LYS
L3698	L3635	D3643	T3399	ILE	LYS	L2932	K2814	ASN	L2598	TYR	SER	L2384	LEU
K3699	S3644	S3644	L3400	ALA	GLU	L2934	H2817	GLY	T2599	ILE	SER	V2388	GLN
D3701	V3636	L3645	L3645	SER	PHE	S2941	T2821	ASP	N2600	GLY	LYS	L2420	ALA
W3702	R3637	P3654	N3403	PRO	HIS	A2942	E2822	ILE	T2601	LEU	ASP	S2602	THR
S3706	S3638	P3654	P3417	ASP	GLY	R2944	E2823	F2684	P2603	GLY	LYS	L2420	SER
E3707	A3640	W3683	N3424	ASN	GLY	V2944	Q2827	N2687	T2604	ILE	GLU	ALA	LYS
V3708	S3641	I3666	S3427	ALA	LEU	SER	Q2827	A2688	L2604	PRO	VAL	PRO	HIS
V3709	P3642	T3667	S3431	E3158	D3028	THR	D2834	N2689	LEU	ALA	ASP	VAL	PHE
F3710	C3643	P3642	T3432	H3199	L3036	THR	D2834	R2690	SER	LYS	GLU	ALA	LYS
L3711	S3645	P3642	T3433	R3193	L3040	THR	K2838	I2691	PRO	PRO	GLU	GLU	ASP
A3714	HIS	P3642	T3433	S3198	L3058	THR	N2847	P2692	THR	PRO	LEU	ALA	ILE
L3715	ILE	P3642	T3433	F3201	L3068	THR	F2848	V2693	GLY	ALA	GLN	MET	ARG
L3716	SER	P3642	T3433	E3242	R3068	THR	V2850	I2694	THR	ASN	ASP	GLY	ARG
F3717	SER	P3642	T3433	D3209	T3074	THR	V2851	N2697	ASP	THR	LEU	GLY	ARG
L3718	GLU	P3642	T3433	E3079	A3094	THR	V2856	Q2698	ASP	GLY	VAL	THR	THR
L3719	SER	P3642	T3433	A3097	A3097	THR	R2880	V2707	LEU	GLY	VAL	VAL	ALA
C3720	ILE	P3642	T3433	N3249	A3097	THR	R2880	L2708	LEU	GLY	ASP	GLY	GLU
H3721	ALA	P3642	T3433	L3220	F3084	THR	V2859	T2714	GLY	GLY	ASP	GLY	THR
SER	GLN	P3642	T3433	I3223	F3084	THR	V2859	L2715	LEU	GLY	ASP	GLY	VAL
GLY	SER	P3642	T3433	H3224	D3093	THR	V2867	L2716	ALA	GLY	ASP	GLY	ASP
THR	ASP	P3642	T3433	E3242	A3094	THR	V2867	R2717	ALA	GLY	ASP	GLY	THR
SER	ASN	P3642	T3433	E3242	A3094	THR	V2867	T2718	ALA	GLY	ASP	GLY	ASP
GLY	TYR	P3642	T3433	E3242	A3094	THR	V2867	W2719	ALA	GLY	ASP	GLY	THR
SER	GLN	P3642	T3433	N3249	A3097	THR	V2867	V2722	THR	GLY	ASP	GLY	GLU
GLN	CYS	P3642	T3433	L3220	F3084	THR	V2867	L2722	GLN	LYS	SER	SER	VAL
ASN	PRO	P3642	T3433	T3255	N3101	THR	V2867	L2729	GLN	ASP	ASP	ASP	THR
LYS	LEU	P3642	T3433	G3102	G3102	THR	V2867	L2729	L2629	PRO	ASP	ASP	THR
LEU	SER	P3642	T3433	G3103	G3103	THR	V2867	L2729	L2630	LEU	LEU	SER	LYS
SER	SER	P3642	T3433	R2881	G3103	THR	V2867	L2729	L2631	ALA	SER	LEU	ALA
SER	THR	P3642	T3433	L3291	I3107	THR	V2867	L2729	Q2632	ALA	GLN	GLN	GLY
THR	THR	P3642	T3433	K3297	R3116	THR	V2867	L2729	L2639	VAL	SER	SER	SER
ASP	ASP	P3642	T3433	T3311	S3124	THR	V2867	L2729	N2640	PHE	SER	SER	PRO
ASP	VAL	P3642	T3433	T3311	M3125	THR	V2867	L2729	F2643	THR	THR	THR	THR
LYS	LYS	P3642	T3433	T3311	V3126	THR	V2867	L2729	N2644	PRO	GLN	ILE	ILE
ASN	ASN	P3642	T3433	T3311	V3126	THR	V2867	L2729	K2645	ILE	LEU	LEU	PRO
ALA	ALA	P3642	T3433	T3311	K3131	THR	V2867	L2729	M2649	SER	SER	LEU	PRO
GLN	GLN	P3642	T3433	T3311	F3132	THR	V2867	L2729	L2650	THR	THR	THR	THR
ALA	ALA	P3642	T3433	T3311	L3133	THR	V2867	L2729	V2655	ASP	ASP	GLY	GLY
PRO	PRO	P3642	T3433	T3311	D3134	THR	V2867	L2729	L2661	TRP	TRP	THR	THR
L3603	L3604	P3642	T3433	T3311	SER	THR	V2867	L2729	Q2662	GLY	GLY	THR	THR
A3604	A3604	P3642	T3433	T3311	GLY	THR	V2867	L2729	L2663	ALA	ALA	THR	THR
L3610	L3610	P3642	T3433	T3311	PRO	THR	V2867	L2729	L2663	ASP	ASP	THR	THR
S3615	S3615	P3642	T3433	T3311	LYS	THR	V2867	L2729	L2663	ASP	ASP	THR	THR
Q3618	Q3618	P3642	T3433	T3311	VAL	THR	V2867	L2729	L2663	ASP	ASP	THR	THR
S3619	S3619	P3642	T3433	T3311	ASP	THR	V2867	L2729	L2663	ASP	ASP	THR	THR
P3620	P3620	P3642	T3433	T3311	SER	THR	V2867	L2729	L2663	ASP	ASP	THR	THR
L3690	L3690	P3642	T3433	T3311	THR	THR	V2867	L2729	L2663	ASP	ASP	THR	THR
T3691	T3691	P3642	T3433	T3311	LEU	THR	V2867	L2729	L2663	ASP	ASP	THR	THR
E3692	E3692	P3642	T3433	T3311	LYS	THR	V2867	L2729	L2663	ASP	ASP	THR	THR
A3622	A3622	P3642	T3433	T3311	THR	THR	V2867	L2729	L2663	ASP	ASP	THR	THR
I3623	I3623	P3642	T3433	T3311	THR	THR	V2867	L2729	L2663	ASP	ASP	THR	THR
V3693	V3693	P3642	T3433	T3311	THR	THR	V2867	L2729	L2663	ASP	ASP	THR	THR

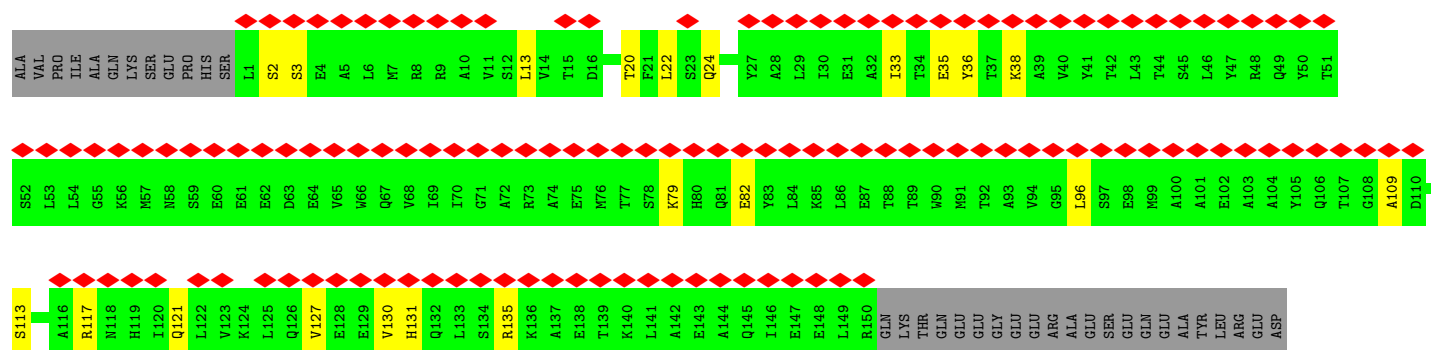


[illegible]

- Molecule 2: Diablo IAP-binding mitochondrial protein



- Molecule 2: Diablo IAP-binding mitochondrial protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36872	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 ($e^-/\text{\AA}^2$)	47.27	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.429	Depositor
Minimum map value	-0.750	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.144	Depositor
Map size (Å)	248.7, 248.7, 248.7	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	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	0.24	0/22620	0.47	0/30734
1	B	0.24	0/22774	0.47	0/30945
2	C	0.23	0/1197	0.46	0/1620
2	D	0.24	0/1197	0.44	0/1620
All	All	0.24	0/47788	0.47	0/64919

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	22195	0	22593	384	0
1	B	22348	0	22749	463	0
2	C	1183	0	1185	23	0
2	D	1183	0	1185	15	0
All	All	46909	0	47712	860	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 9.

The worst 5 of 860 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:1818:ASP:HB2	1:B:1857:LYS:HB3	1.62	0.81
1:B:1032:GLU:HB3	1:B:1307:LYS:HG3	1.66	0.76
1:A:1052:GLU:OE1	1:A:1056:ARG:NH1	2.17	0.76
1:A:1103:HIS:O	1:A:1305:ARG:NH2	2.18	0.76
1:A:1806:ILE:HG12	1:A:1876:GLY:HA3	1.68	0.75

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	2799/4859 (58%)	2712 (97%)	87 (3%)	0	100	100
1	B	2820/4859 (58%)	2741 (97%)	79 (3%)	0	100	100
2	C	148/184 (80%)	146 (99%)	2 (1%)	0	100	100
2	D	148/184 (80%)	147 (99%)	1 (1%)	0	100	100
All	All	5915/10086 (59%)	5746 (97%)	169 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2517/4217 (60%)	2509 (100%)	8 (0%)	92	97
1	B	2534/4217 (60%)	2523 (100%)	11 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	128/157 (82%)	127 (99%)	1 (1%)	81	93
2	D	128/157 (82%)	128 (100%)	0	100	100
All	All	5307/8748 (61%)	5287 (100%)	20 (0%)	91	97

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3131	LYS
1	B	3779	LYS
2	C	9	ARG
1	B	3970	LYS
1	A	4218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1058	HIS
1	B	2370	HIS
1	B	3997	GLN
1	B	3493	HIS
1	B	3790	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.

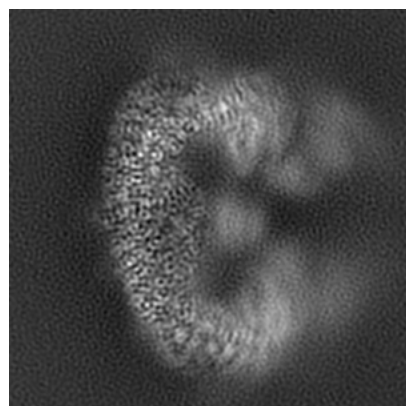
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15654. These allow visual inspection of the internal detail of the map and identification of artifacts.

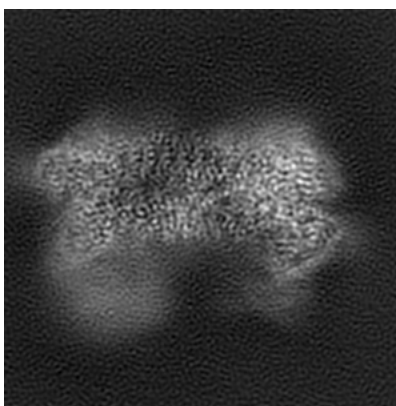
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

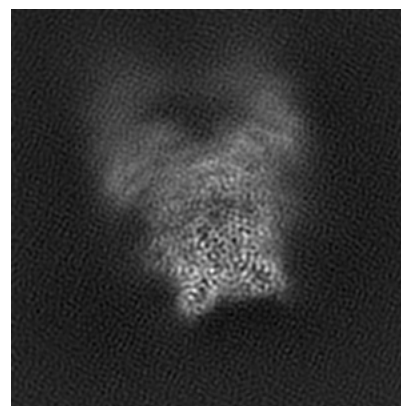
6.1.1 Primary map



X

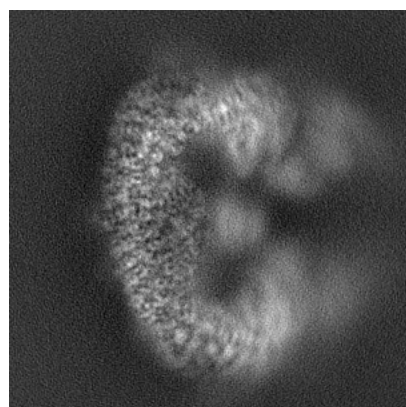


Y

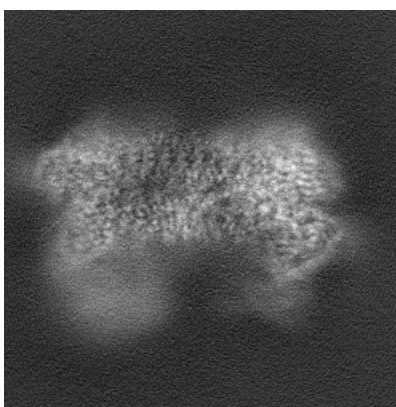


Z

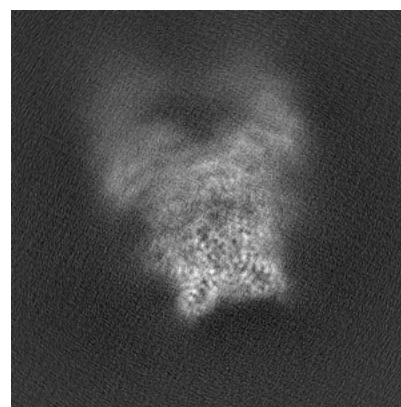
6.1.2 Raw map



X



Y

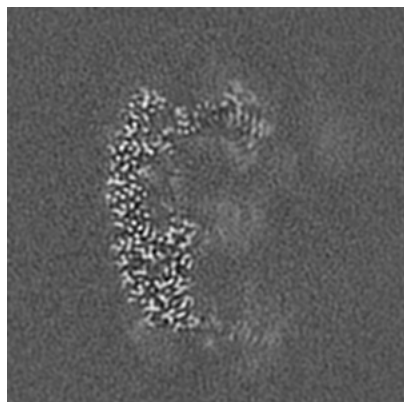


Z

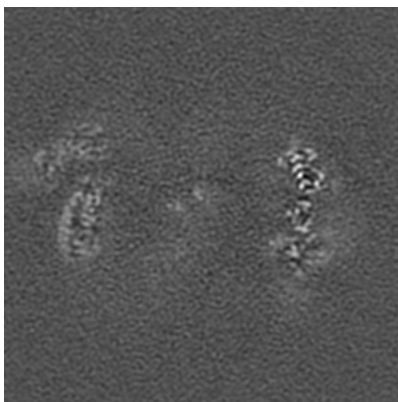
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

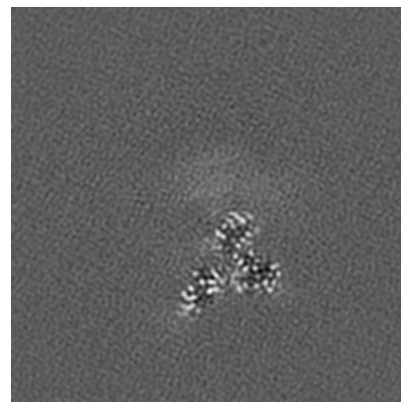
6.2.1 Primary map



X Index: 150

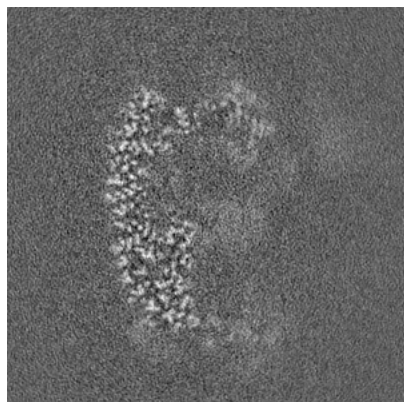


Y Index: 150

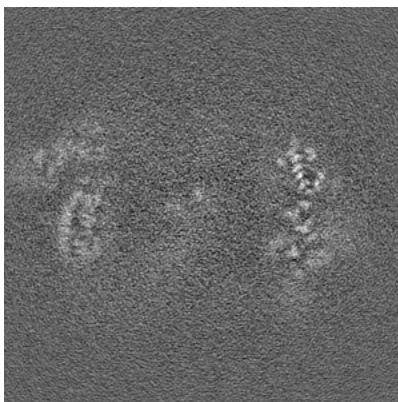


Z Index: 150

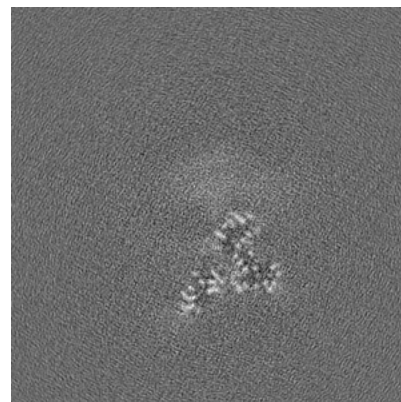
6.2.2 Raw map



X Index: 150



Y Index: 150

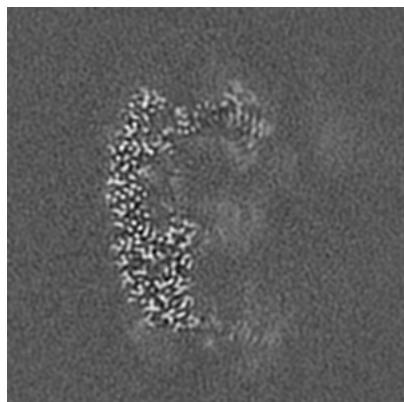


Z Index: 150

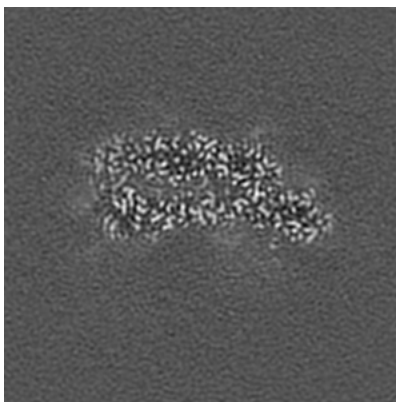
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

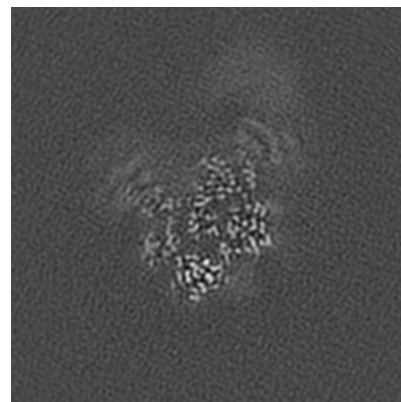
6.3.1 Primary map



X Index: 150

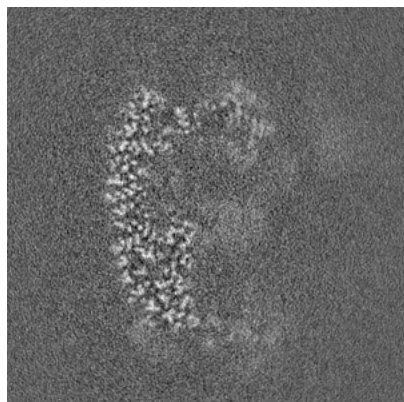


Y Index: 99

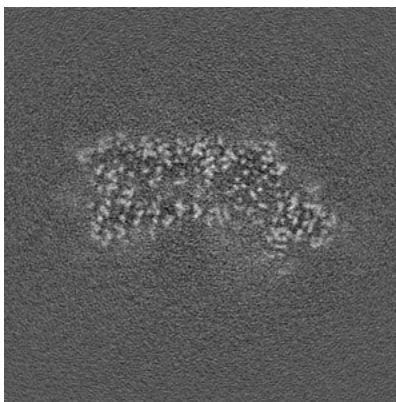


Z Index: 217

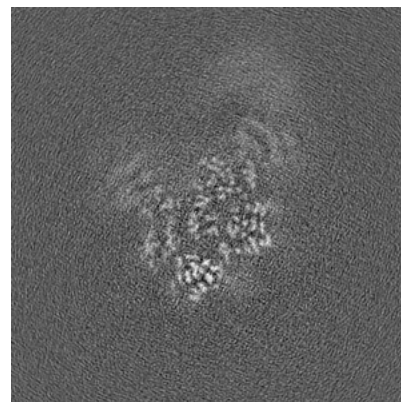
6.3.2 Raw map



X Index: 150



Y Index: 104

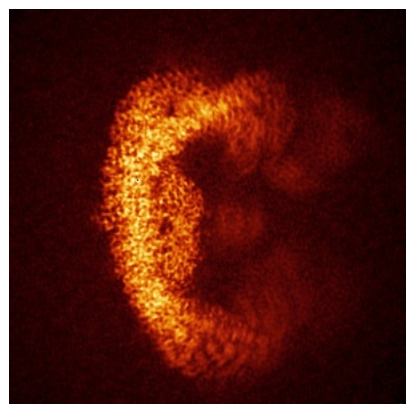


Z Index: 217

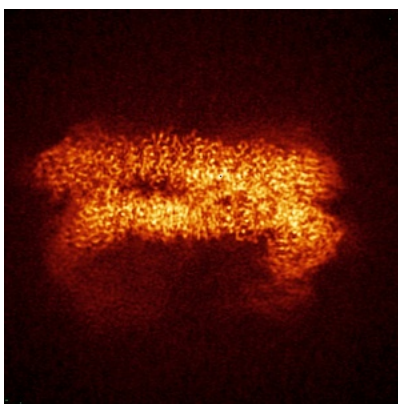
The images above show the largest variance slices of the map in three orthogonal directions.

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

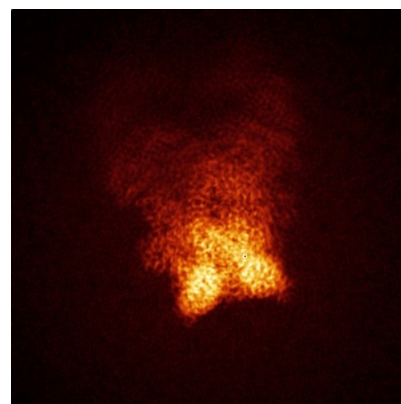
6.4.1 Primary map



X

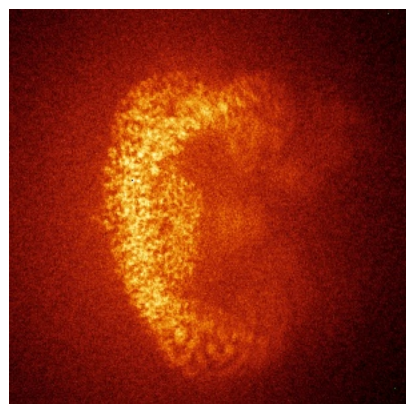


Y

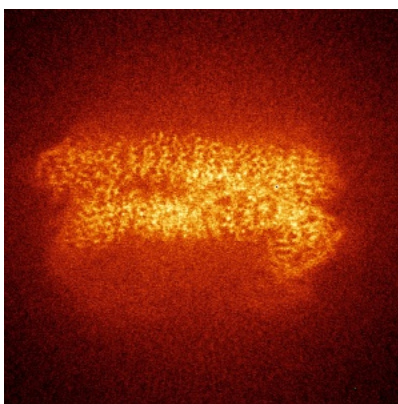


Z

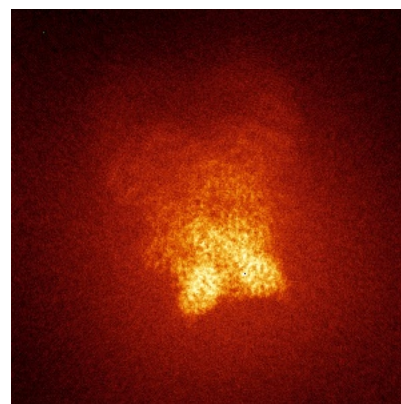
6.4.2 Raw map



X



Y

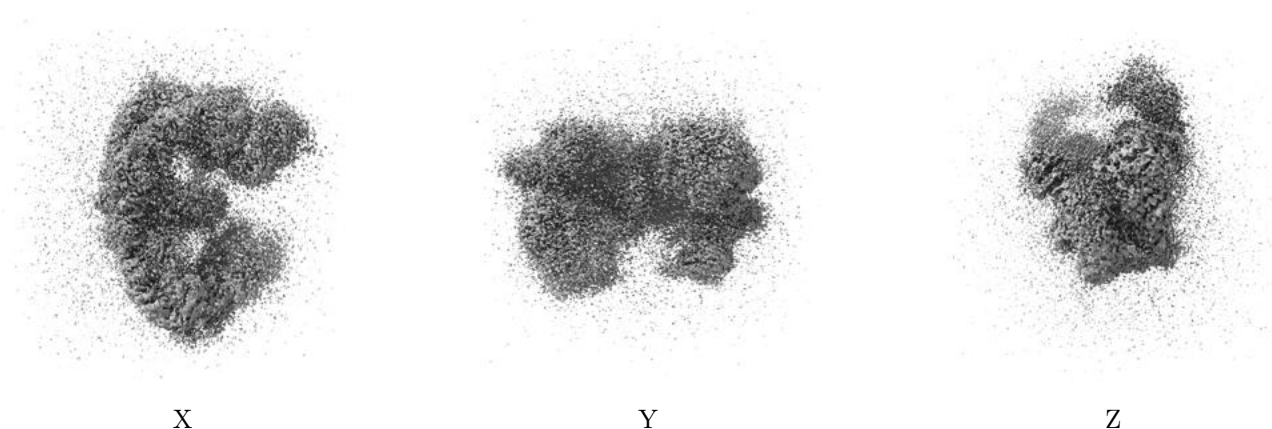


Z

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.

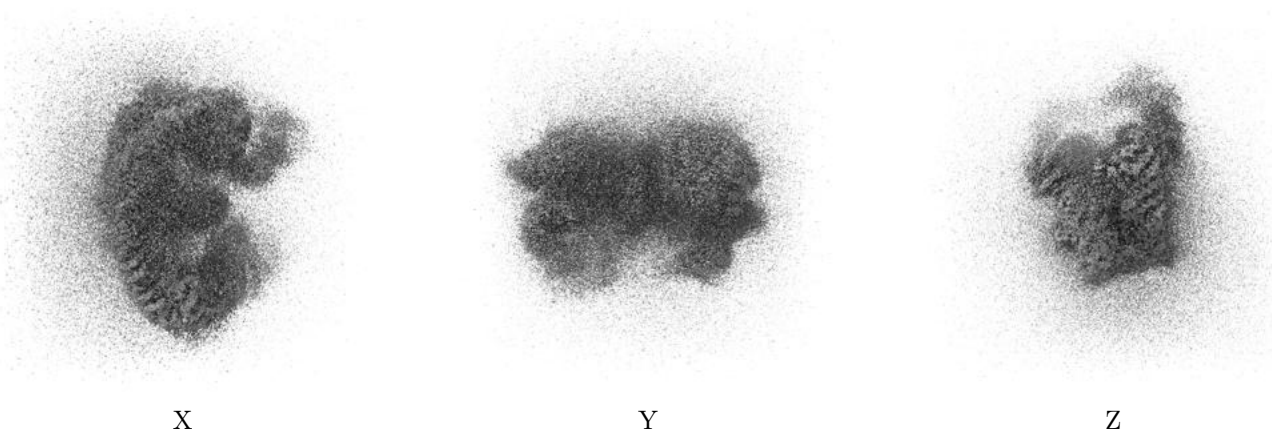
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.144. 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.

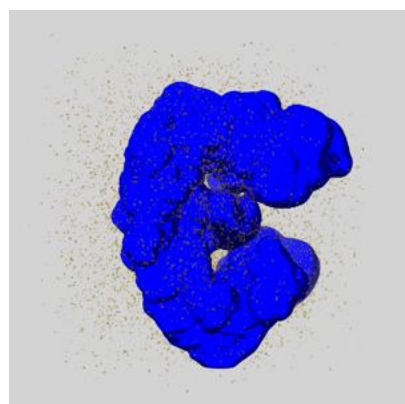
6.6 Mask visualisation [i](#)

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

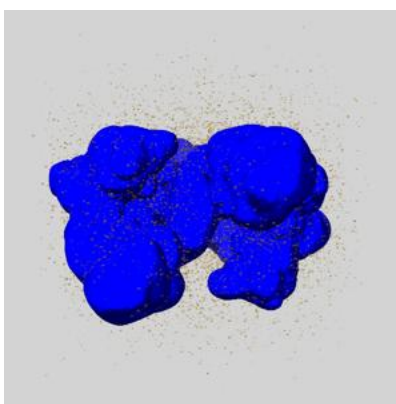
A mask typically either:

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

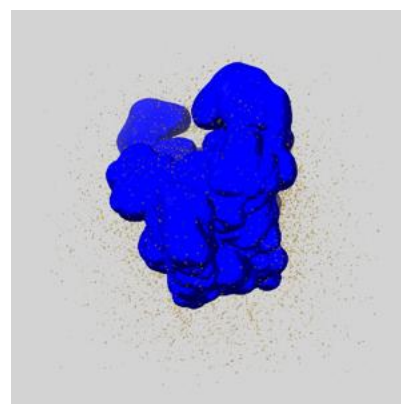
6.6.1 emd_15654_msk_1.map [i](#)



X



Y

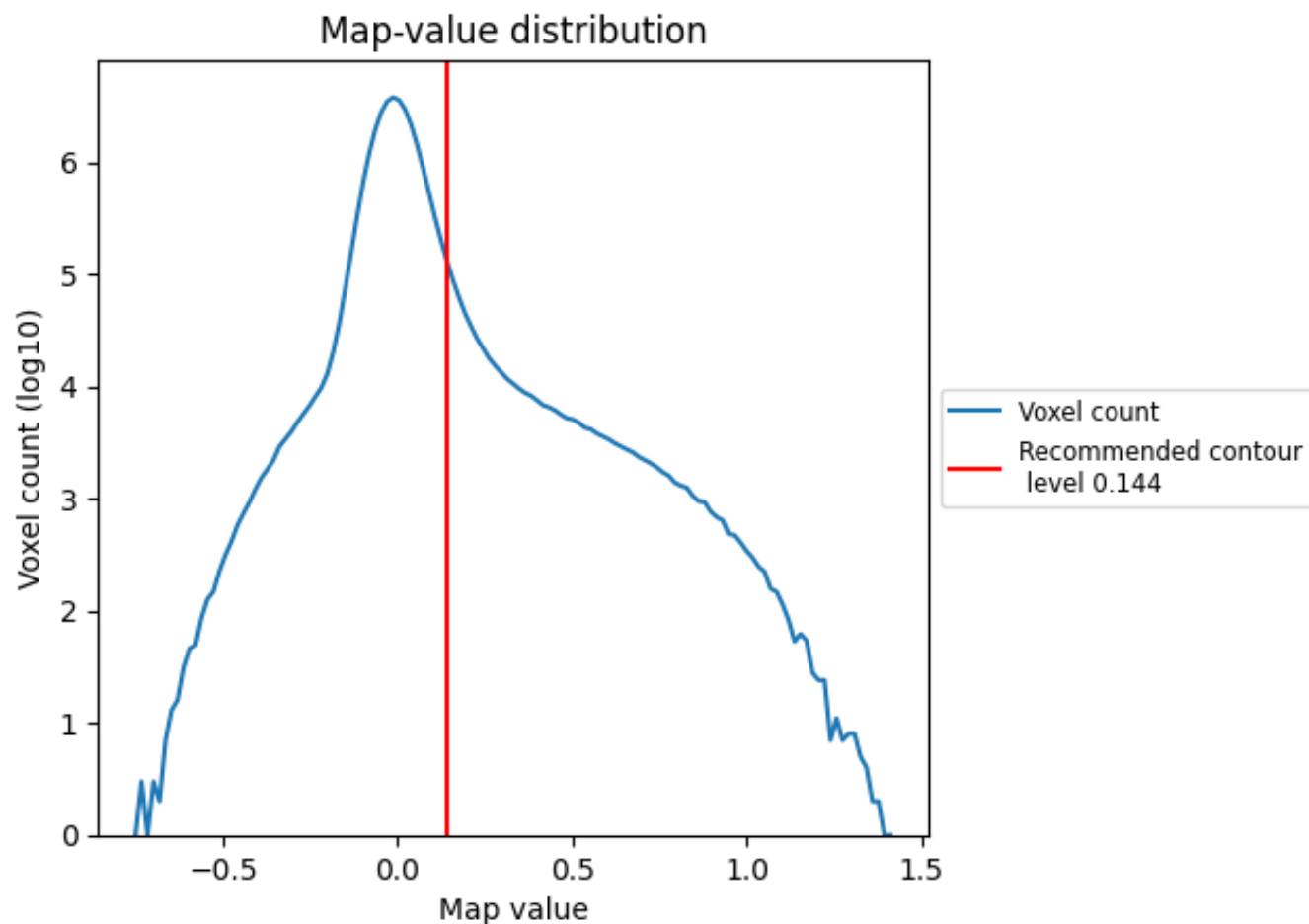


Z

7 Map analysis [i](#)

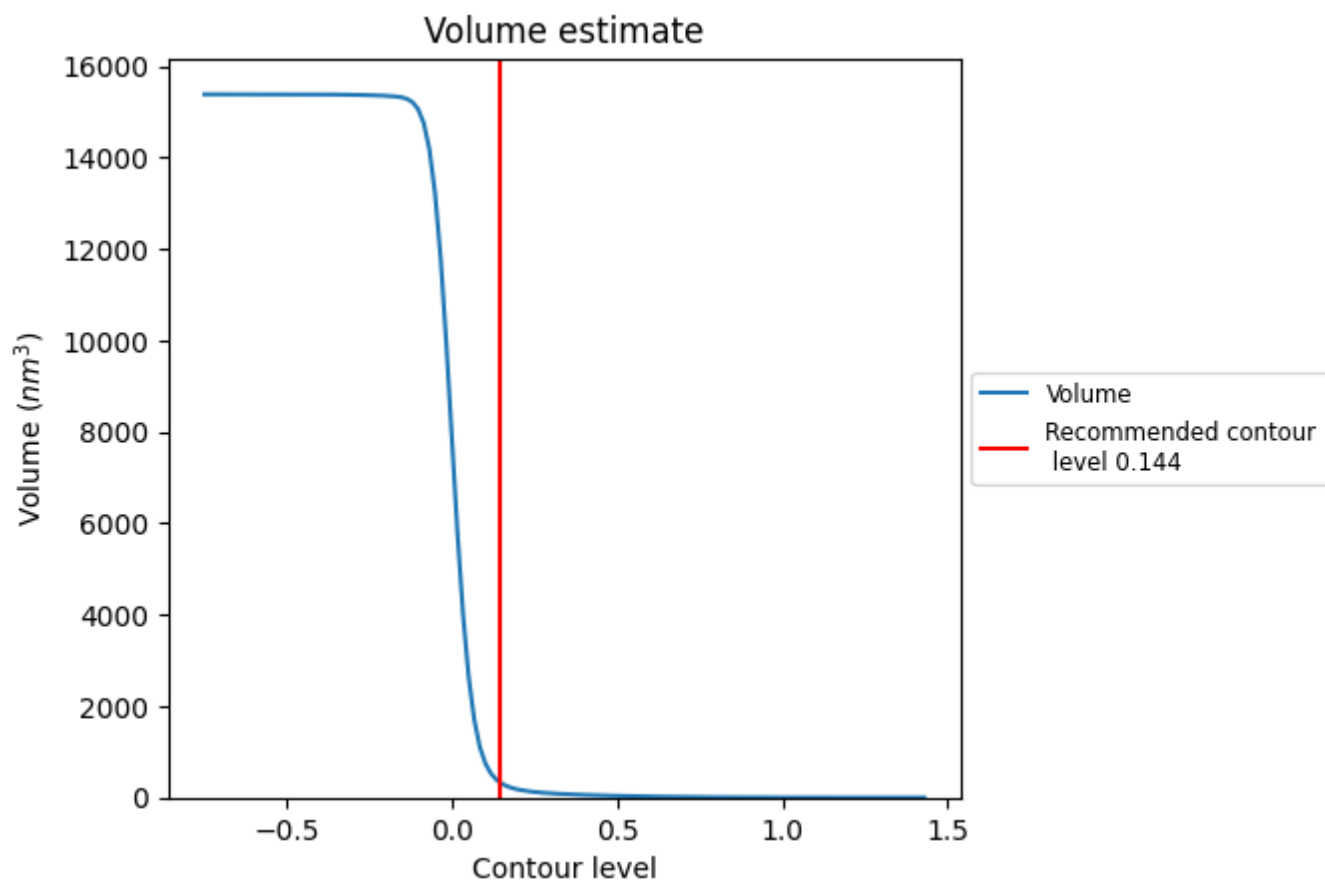
This section contains the results of statistical analysis of the map.

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.

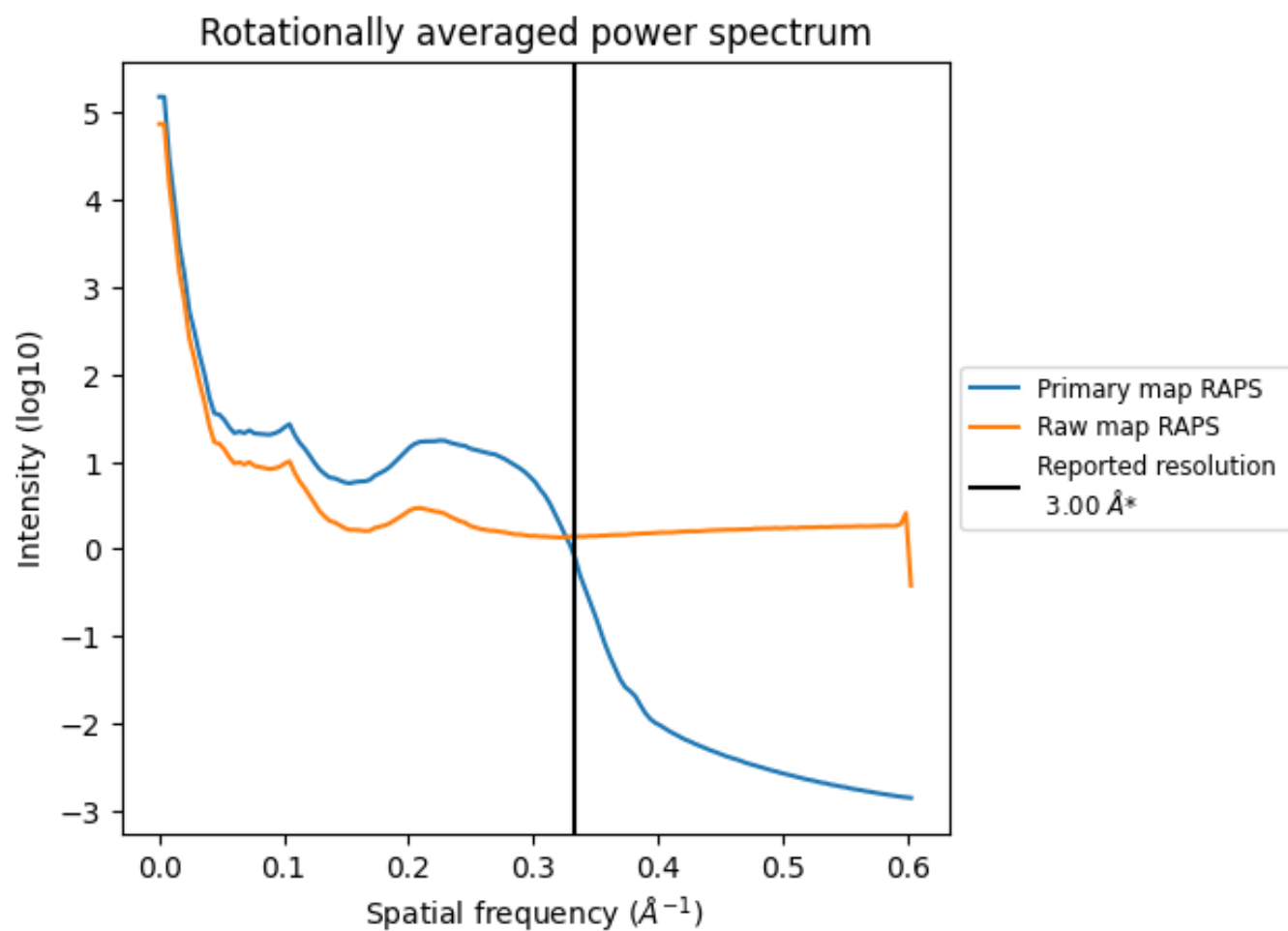
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 339 nm³; this corresponds to an approximate mass of 307 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 ⓘ

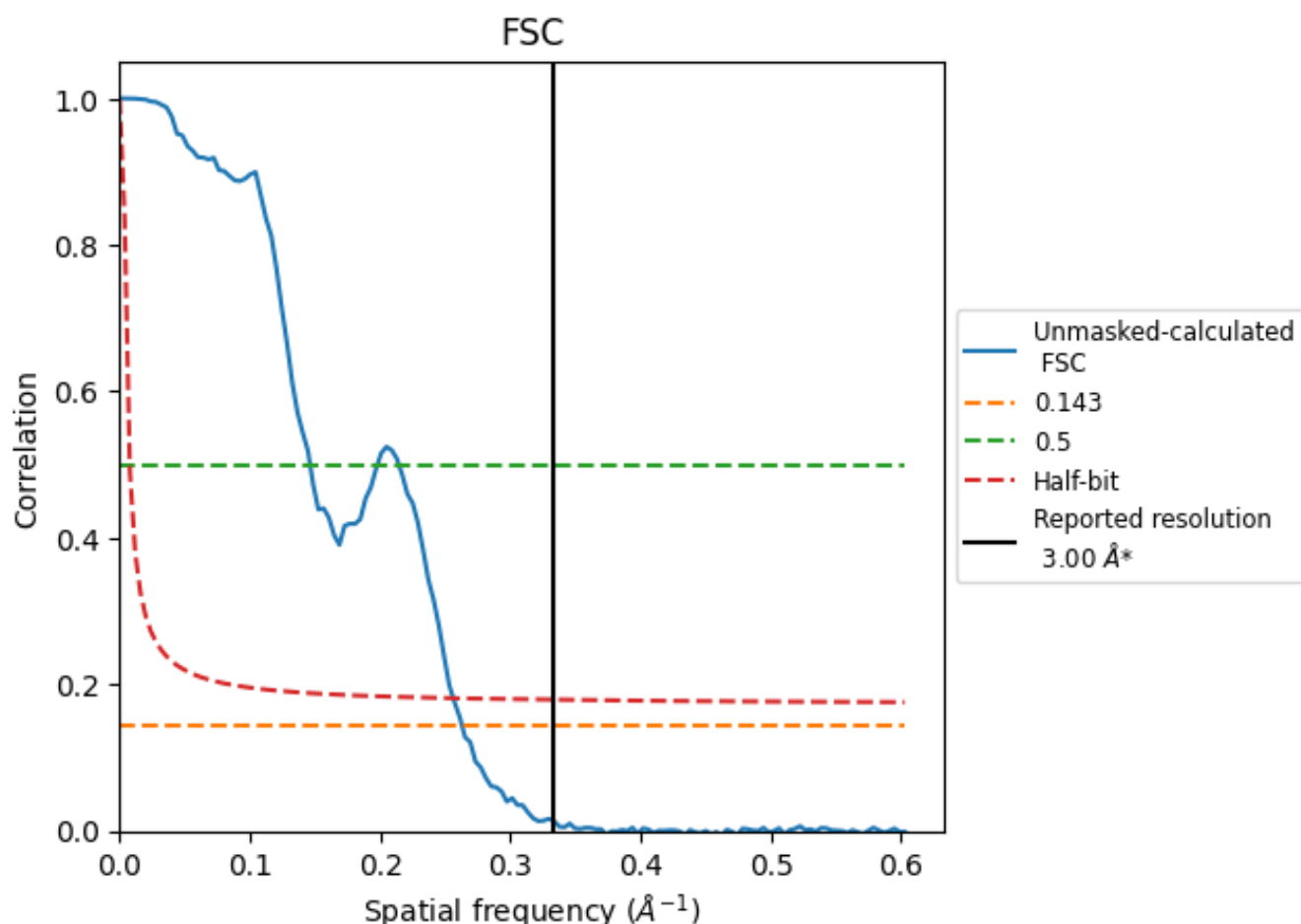


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

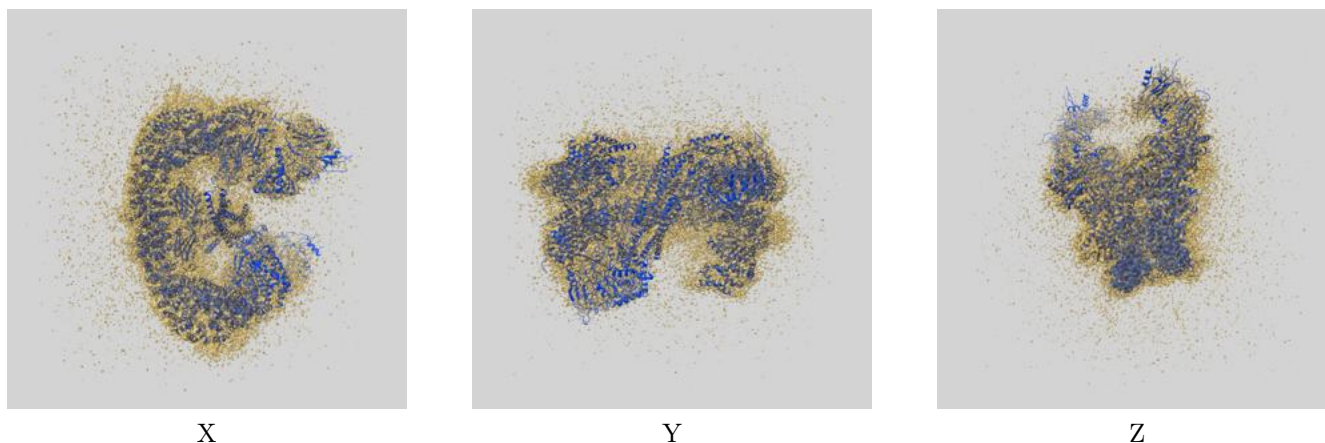
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	6.83	3.90

*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 3.80 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

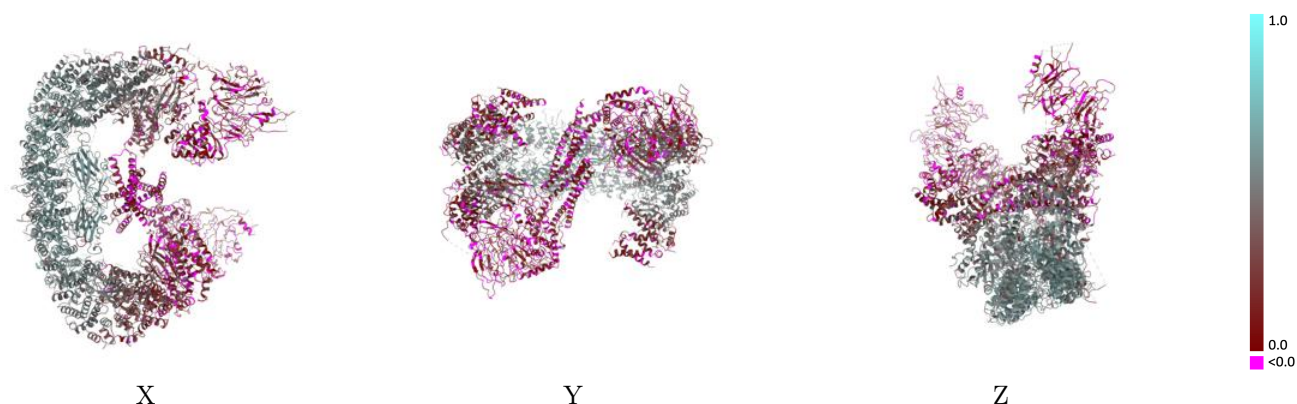
This section contains information regarding the fit between EMDB map EMD-15654 and PDB model 8ATO. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



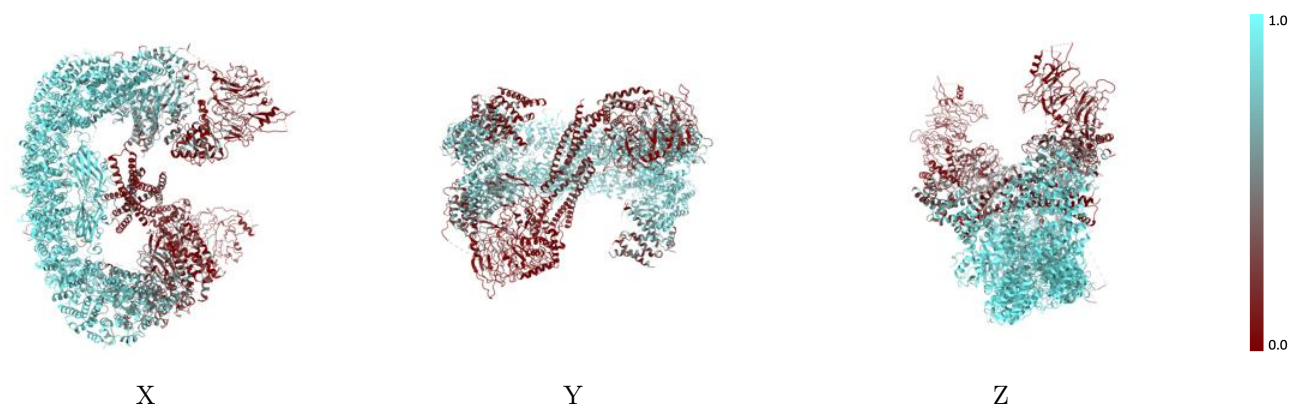
The images above show the 3D surface view of the map at the recommended contour level 0.144 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



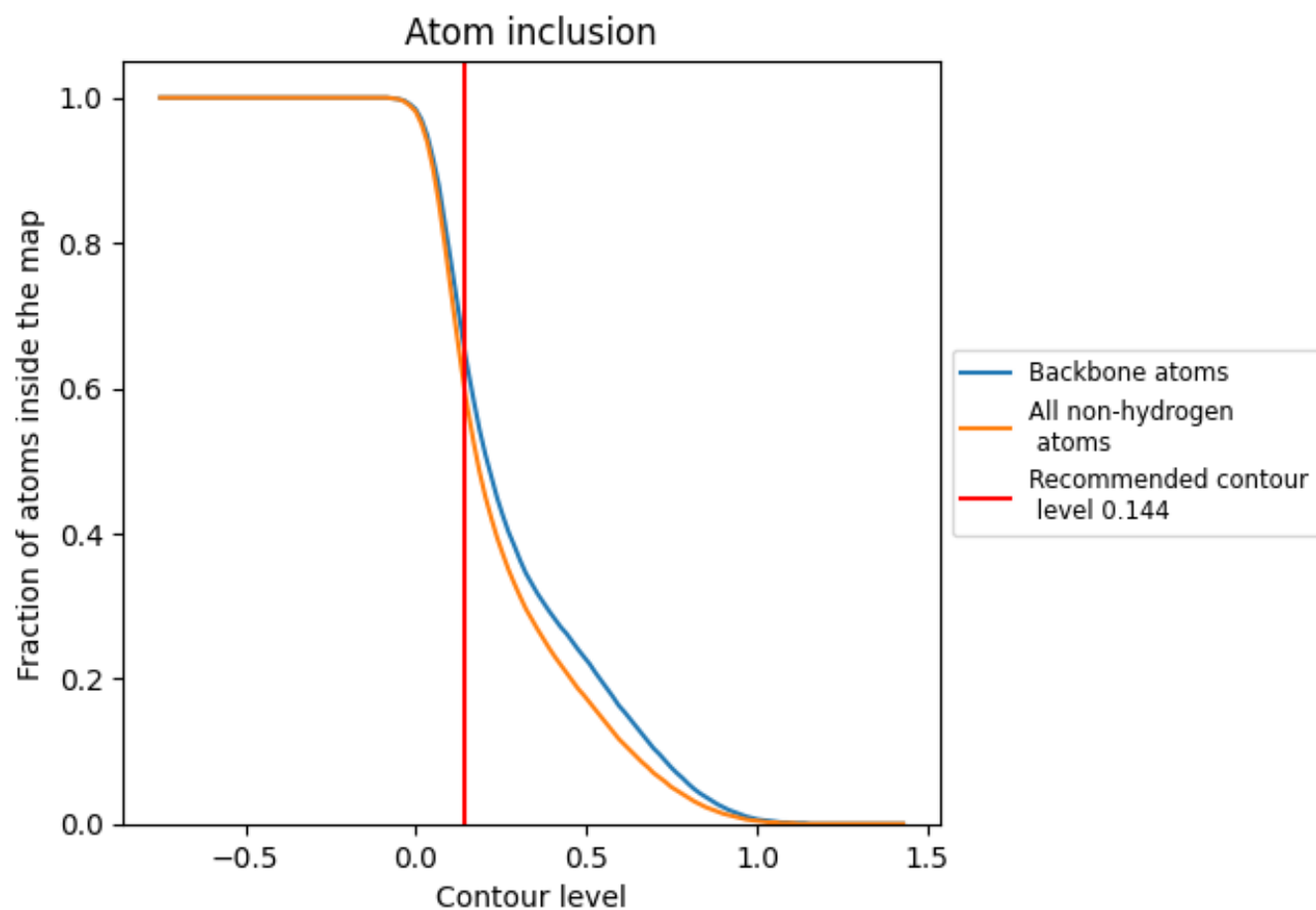
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.144).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 59% 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 (0.144) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5930	<div></div> 0.3340
A	<div></div> 0.5920	<div></div> 0.3390
B	<div></div> 0.6390	<div></div> 0.3550
C	<div></div> 0.1930	<div></div> 0.0830
D	<div></div> 0.1490	<div></div> 0.0780

