



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 12:28 PM UTC

PDB ID : 7MWE / pdb_00007mwe
EMDB ID : EMD-22429
Title : HUWE1 in map with focus on WWE
Authors : Hunkeler, M.; Fischer, E.S.
Deposited on : 2021-05-16
Resolution : 3.40 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.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

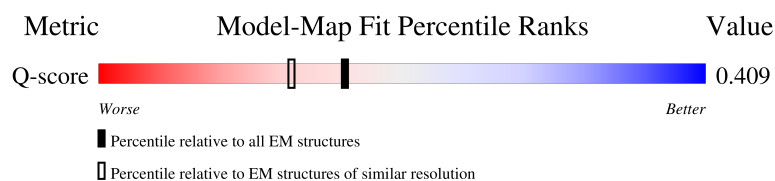
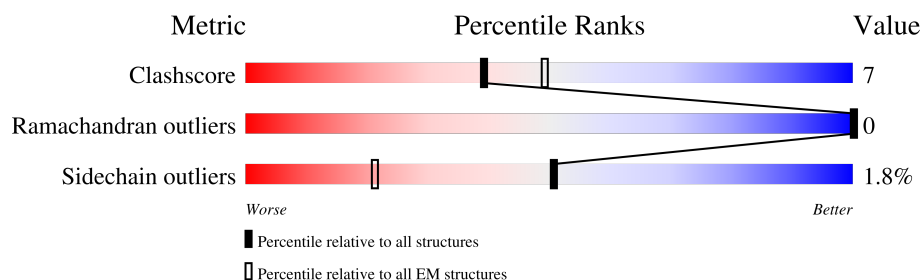
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	4411	13% 45% 10% 45%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 38719 atoms, of which 19554 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 E3 ubiquitin-protein ligase HUWE1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2427	Total	C	H	N	O	S	0	0
			38719	12225	19554	3292	3528	120		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-36	MET	-	expression tag	UNP Q7Z6Z7
A	-35	ASP	-	expression tag	UNP Q7Z6Z7
A	-34	TYR	-	expression tag	UNP Q7Z6Z7
A	-33	LYS	-	expression tag	UNP Q7Z6Z7
A	-32	ASP	-	expression tag	UNP Q7Z6Z7
A	-31	ASP	-	expression tag	UNP Q7Z6Z7
A	-30	ASP	-	expression tag	UNP Q7Z6Z7
A	-29	ASP	-	expression tag	UNP Q7Z6Z7
A	-28	LYS	-	expression tag	UNP Q7Z6Z7
A	-27	LEU	-	expression tag	UNP Q7Z6Z7
A	-26	ALA	-	expression tag	UNP Q7Z6Z7
A	-25	ALA	-	expression tag	UNP Q7Z6Z7
A	-24	ALA	-	expression tag	UNP Q7Z6Z7
A	-23	ASN	-	expression tag	UNP Q7Z6Z7
A	-22	SER	-	expression tag	UNP Q7Z6Z7
A	-21	SER	-	expression tag	UNP Q7Z6Z7
A	-20	ILE	-	expression tag	UNP Q7Z6Z7
A	-19	ASP	-	expression tag	UNP Q7Z6Z7
A	-18	LEU	-	expression tag	UNP Q7Z6Z7
A	-17	ILE	-	expression tag	UNP Q7Z6Z7
A	-16	SER	-	expression tag	UNP Q7Z6Z7
A	-15	THR	-	expression tag	UNP Q7Z6Z7
A	-14	SER	-	expression tag	UNP Q7Z6Z7
A	-13	LEU	-	expression tag	UNP Q7Z6Z7
A	-12	TYR	-	expression tag	UNP Q7Z6Z7
A	-11	LYS	-	expression tag	UNP Q7Z6Z7
A	-10	LYS	-	expression tag	UNP Q7Z6Z7
A	-9	ALA	-	expression tag	UNP Q7Z6Z7

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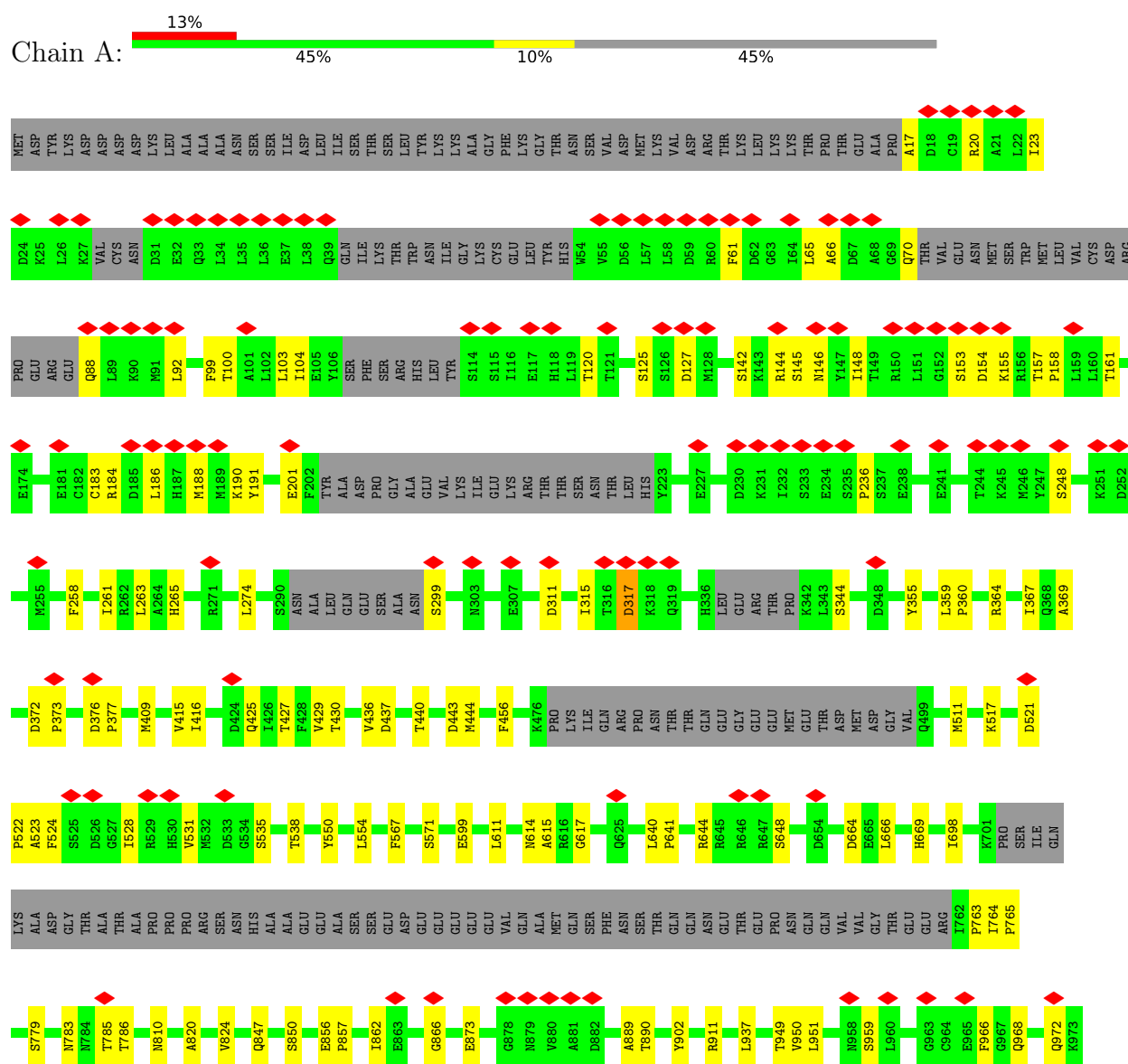
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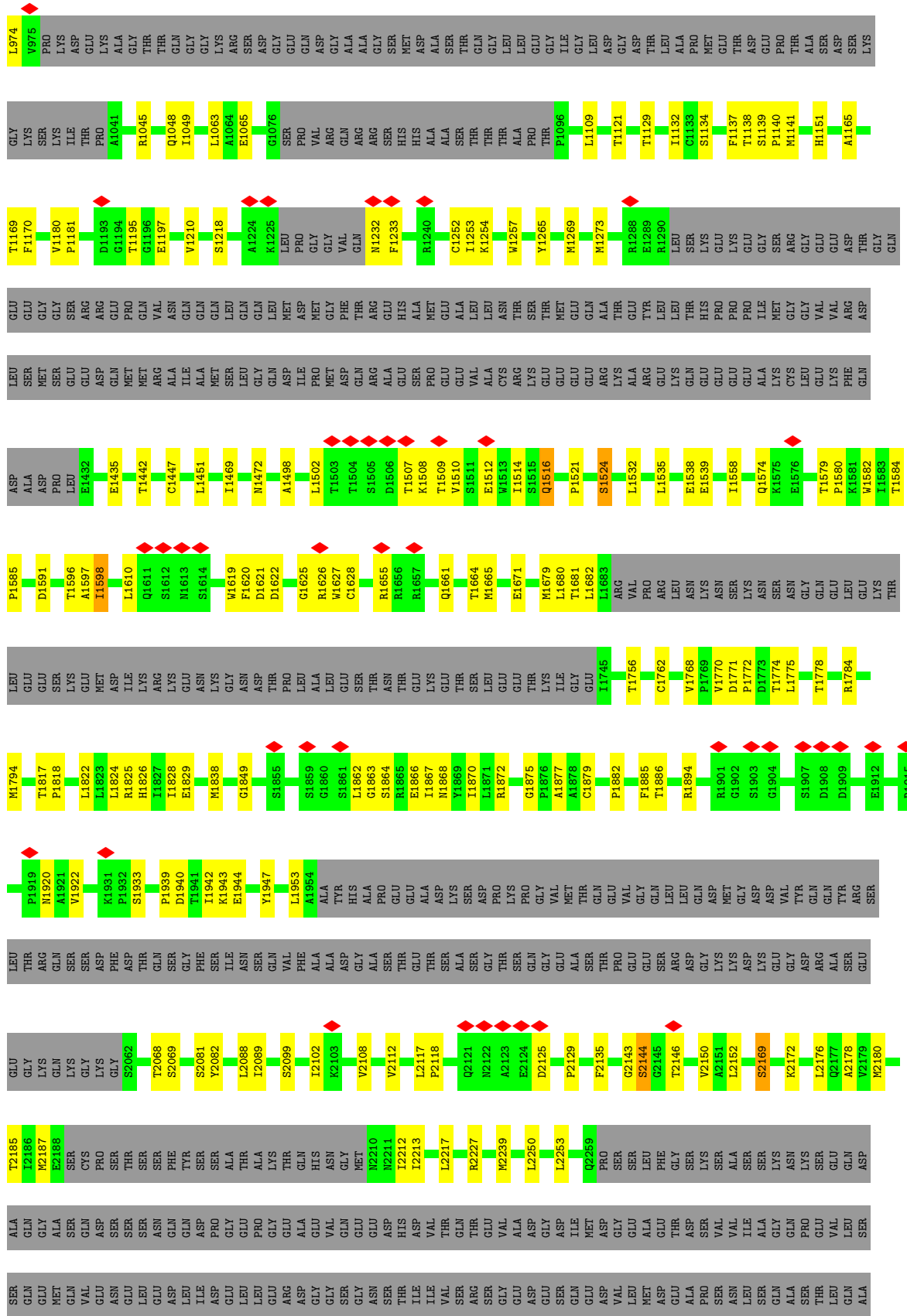
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP Q7Z6Z7
A	-7	PHE	-	expression tag	UNP Q7Z6Z7
A	-6	LYS	-	expression tag	UNP Q7Z6Z7
A	-5	GLY	-	expression tag	UNP Q7Z6Z7
A	-4	THR	-	expression tag	UNP Q7Z6Z7
A	-3	ASN	-	expression tag	UNP Q7Z6Z7
A	-2	SER	-	expression tag	UNP Q7Z6Z7
A	-1	VAL	-	expression tag	UNP Q7Z6Z7
A	0	ASP	-	expression tag	UNP Q7Z6Z7

3 Residue-property plots [i](#)

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: E3 ubiquitin-protein ligase HUWE1







M4317	M4318	G4319	I4320	D4261	L4262	K4263	S4264	M4265	T4266	E4267	Y4268	D4269	K4270	Y4271	Q4272	S4273	R4274	S4275	I4276	Q4277	I4278	Q4279	W4280	F4281	W4282	R4283	A4284	L4285	R4286	S4287	F4288	D4289	Q4290	A4291	D4292	R4293	A4294	K4295	F4296	L4297	Q4298	F4299	V4300	T4301	G4302	T4303	S4304	K4305	V4306	P4307	L4308	Q4309	G4310	F4311	A4312	A4313	L4314	E4315	G4316																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
LEU	V4198	T4199	E4200	E4201	M4202	K4203	K4204	E4205	V4206	W4207	H4208	L4209	W4210	Q4211	Q4212	M4213	R4214	M4215	T4216	G4217	A4218	I4219	K4221	Q4222	L4223	A4224	A4225	F4226	L4227	E4228	Q4229	F4230	Y4231	E4232	I4233	L4234	P4235	K4236	M4237	L4238	I4239	S4240	I4241	F4242	T4243	E4244	Q4245	E4246	L4247	E4248	L4249	L4250	I4251	S4252	Q4253	L4254	P4255	T4256																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
L4137	G4138	K4139	S4140	V4141	R4142	T4143	T4144	D4145	M4146	E4147	S4148	E4149	D4150	Y4151	H4152	F4153	Y4154	Q4155	G4156	L4157	V4158	Y4159	L4160	L4161	E4162	M4163	D4164	V4165	S4166	T4167	L4168	G4169	Y4170	D4171	L4172	T4173	F4174	S4175	T4176	E4177	V4178	Q4179	E4180	F4181	G4182	V4183	C4184	E4185	V4186	R4187	D4188	L4189	K4190	PRO	ASN	GLY	ALA	ASN	ILE																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
M4077	Y4078	A4079	L4080	F4081	R4082	T4083	S4084	P4085	G4086	D4087	R4088	Y4089	T4090	Y4091	T4092	I4093	M4094	P4095	S4096	S4097	H4098	C4099	M4100	P4101	M4102	H4103	L4104	S4105	Y4106	F4107	K4108	F4109	V4110	G4111	R4112	I4113	V4114	A4115	K4116	A4117	V4118	Y4119	D4120	M4121	R4122	L4123	L4124	E4125	C4126	Y4127	F4128	T4129	R4130	S4131	F4132	Y4133	K4134	H4135	I4136																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
M4017	A4018	Y4019	H4020	Y4021	R4022	R4023	D4024	H4025	Y4026	F4027	E4028	D4029	S4030	Y4031	R4032	E4033	L4034	H4035	R4036	K4037	S4038	P4039	E4040	E4041	M4042	K4043	M4044	R4045	L4046	Y4047	I4048	V4049	F4050	E4051	G4052	E4053	E4054	G4055	Q4056	D4057	A4058	G4059	G4060	M4061	L4062	R4063	E4064	Y4065	Y4066	M4067	E4068	I4069	S4070	R4071	E4072	M4073	F4074	M4075	P4076																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
L3956	R3957	F3958	A3959	E3960	T3963	T3964	V3965	L3966	N3967	Q3968	I3969	L3970	R3971	Q3972	S3973	T3974	T3975	H3976	L3977	A3978	D3979	Q3980	F3981	F3982	A3983	V3984	L3985	V3986	D3987	Y3988	I3989	R3990	V3991	L3992	D3993	F3994	D3995	V3996	K3997	R3998	K3999	Y4000	F4001	R4002	Q4003	E4004	L4005	E4006	R4007	L4008	D4009	E4010	G4011	L4012	R4013	E4014	E4015	D4016																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
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SER	ILE	GLN	ALA	ALA	VAL	GLN	GLU	ALA	VAL	ILE	VAL	ASP	ALA	ILE	ILE	LYS	ARG	PRO	GLY	ARG	GLN	ALA	ALA	ALA	THR	SER	GLU	SER	GLU	GLN	ASN	VAL	ARG	GLU	SER	VAL	ASP	GLN	PRO	GLY	GLY	LEU	PRO	SER	PRO	SER	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
GLN	ASP	THR	GLN	ILE	ALA	SER	ASP	THR	GLY	PRO	GLN	GLY	LYS	LYS	GLU	GLU	GLU	GLU	LEU	PRO	LEU	LEU	GLU	GLN	L3851	S3852	L3853	D3854	W3857	D3858	M3859	K3865	E3868	E3869	S3870	H3871	D3872	Q3873	H3874	A3875	V3876	L3877	F3887	L3888	V3889	T3892	E3893	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	85184	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; standard correction in Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.68	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0165	Depositor
Map size ($\text{\AA}$)	300.3, 300.3, 300.3	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.825, 0.825, 0.825	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	0.26	0/19509	0.54	1/26411 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1598	ILE	N-CA-C	-7.94	101.97	110.23

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	19165	19554	19539	280	0
All	All	19165	19554	19539	280	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 7.

The worst 5 of 280 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4023:ARG:O	1:A:4023:ARG:NH1	2.13	0.82
1:A:1109:LEU:HD22	1:A:1138:THR:HG22	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4082:ARG:NH1	1:A:4094:ASN:OD1	2.20	0.75
1:A:1134:SER:O	1:A:1138:THR:HG23	1.87	0.73
1:A:1825:ARG:NH1	1:A:2081:SER:OG	2.21	0.73

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	2369/4411 (54%)	2312 (98%)	57 (2%)	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	2149/3839 (56%)	2111 (98%)	38 (2%)	51	67

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3615	THR
1	A	4183	VAL
1	A	3619	VAL

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Mol	Chain	Res	Type
1	A	3984	VAL
1	A	4327	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4135	HIS
1	A	4343	ASN
1	A	859	HIS
1	A	1255	ASN
1	A	1667	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 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.

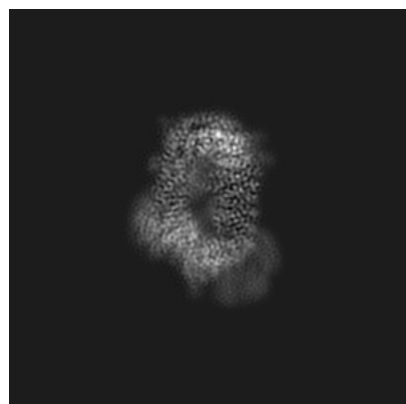
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22429. These allow visual inspection of the internal detail of the map and identification of artifacts.

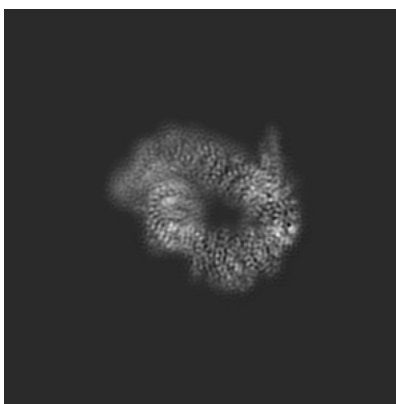
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

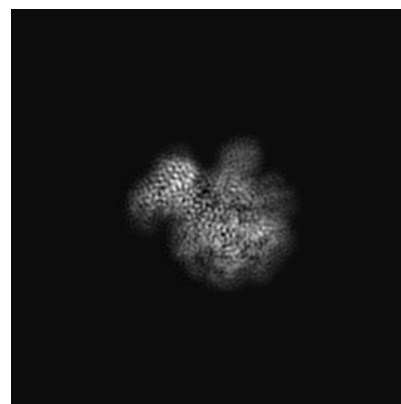
6.1.1 Primary map



X

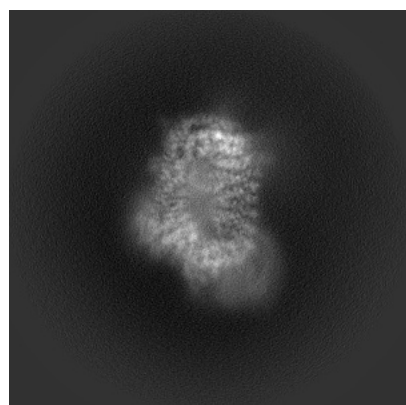


Y

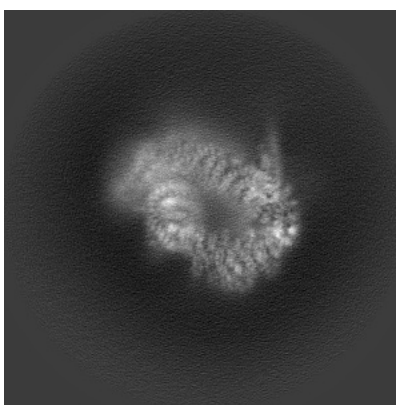


Z

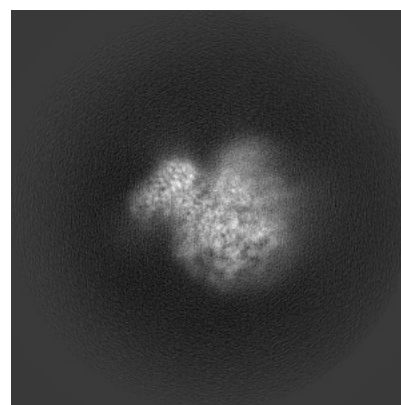
6.1.2 Raw map



X



Y

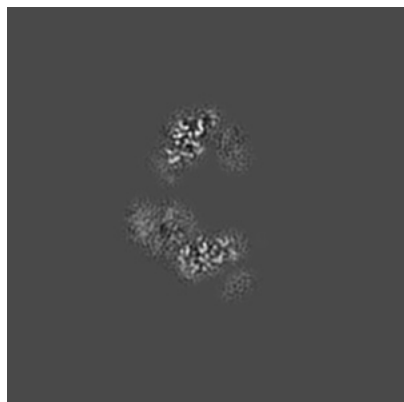


Z

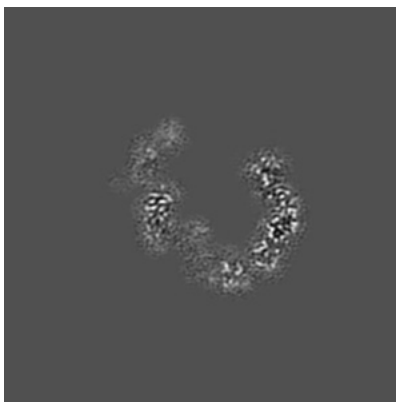
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

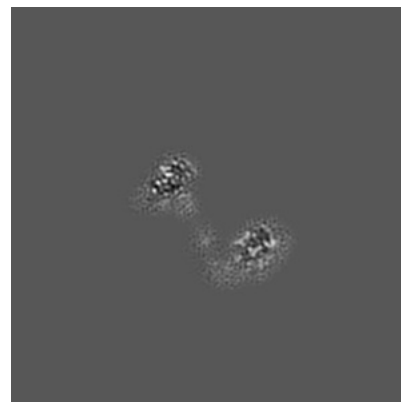
6.2.1 Primary map



X Index: 182

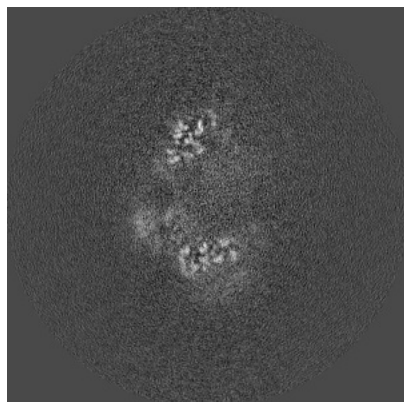


Y Index: 182

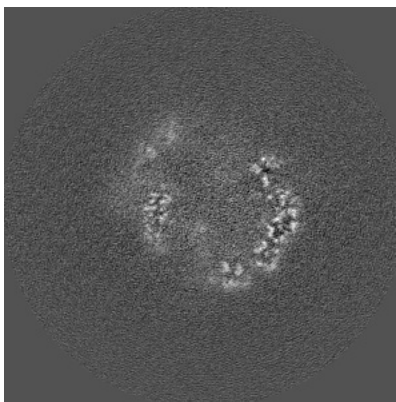


Z Index: 182

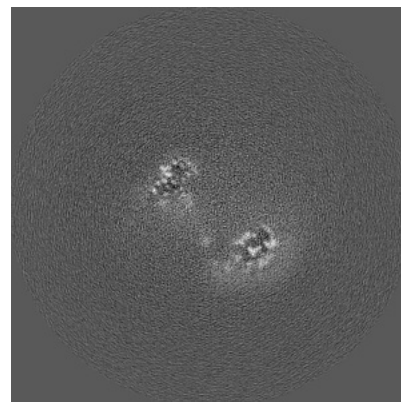
6.2.2 Raw map



X Index: 182



Y Index: 182



Z Index: 182

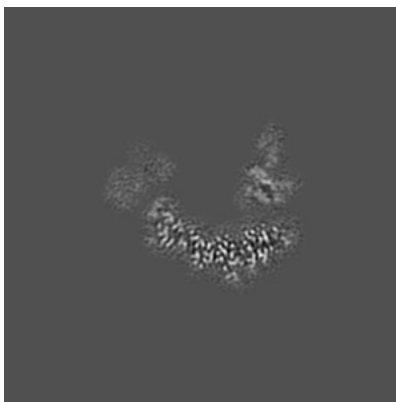
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

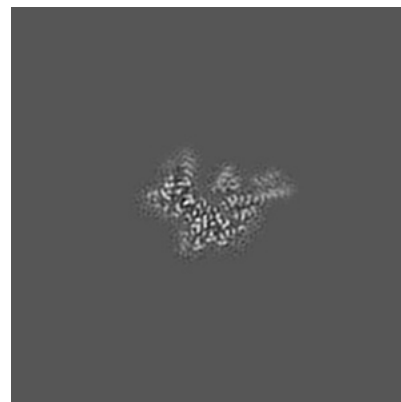
6.3.1 Primary map



X Index: 149

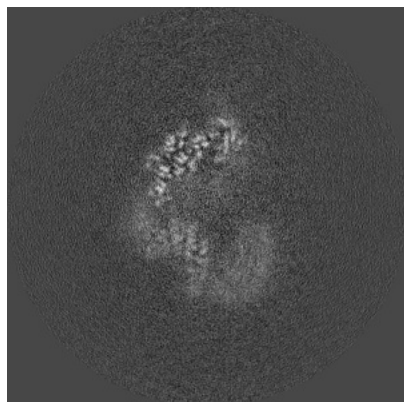


Y Index: 204

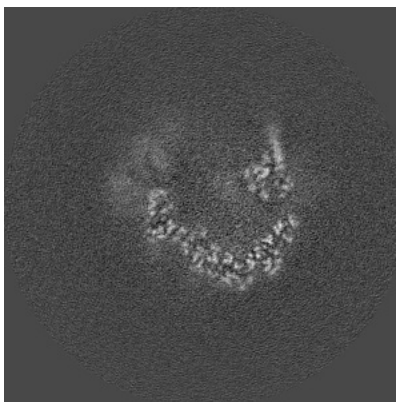


Z Index: 247

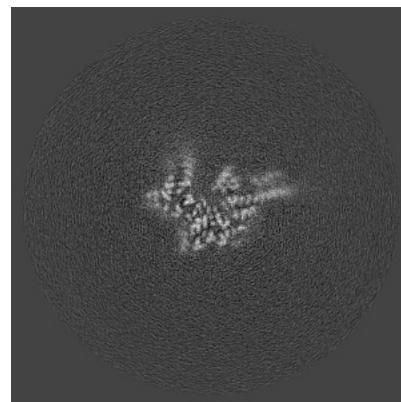
6.3.2 Raw map



X Index: 202



Y Index: 192

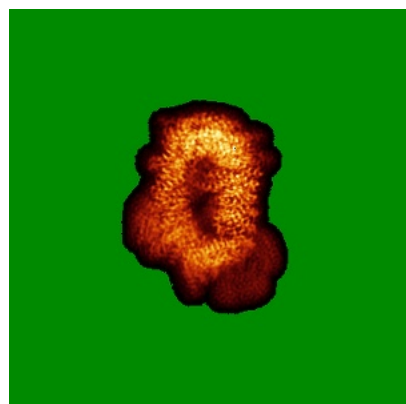


Z Index: 247

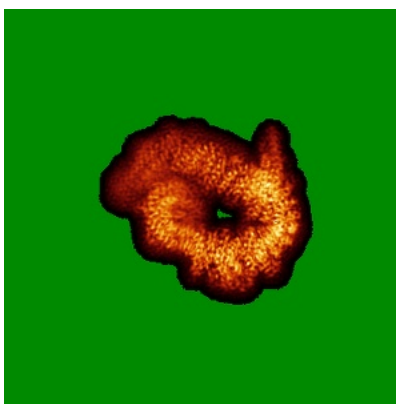
The images above show the largest variance slices of the map in three orthogonal directions.

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

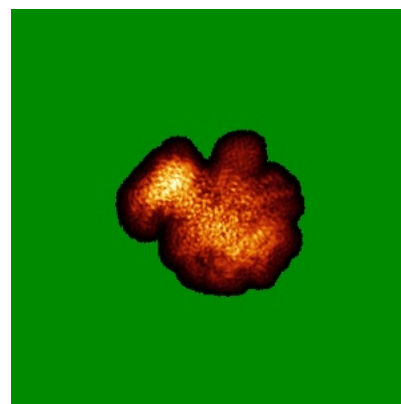
6.4.1 Primary map



X

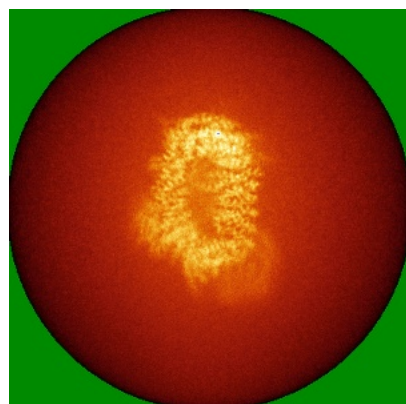


Y

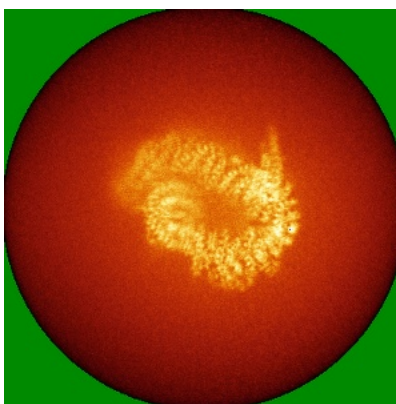


Z

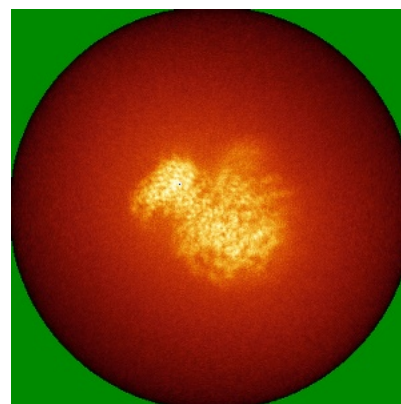
6.4.2 Raw map



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](#)

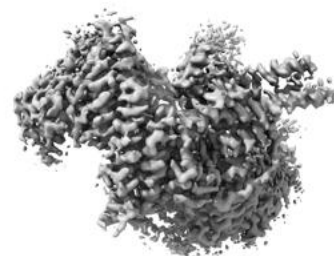
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0165. 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



X



Y



Z

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.

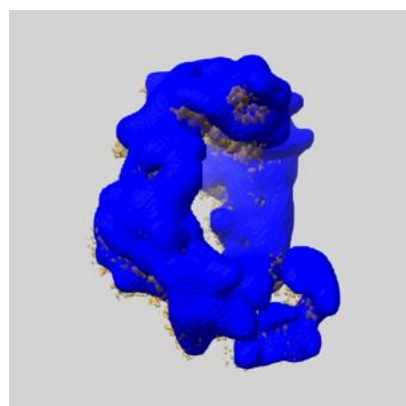
6.6 Mask visualisation [i](#)

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

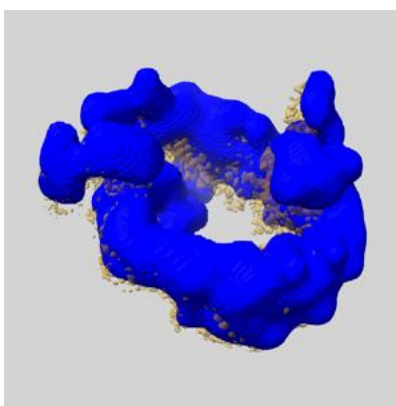
A mask typically either:

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

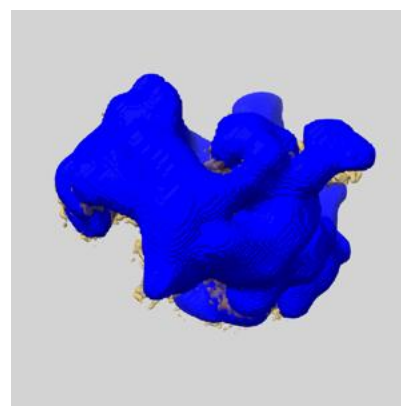
6.6.1 emd_22429_msk_1.map [i](#)



X



Y

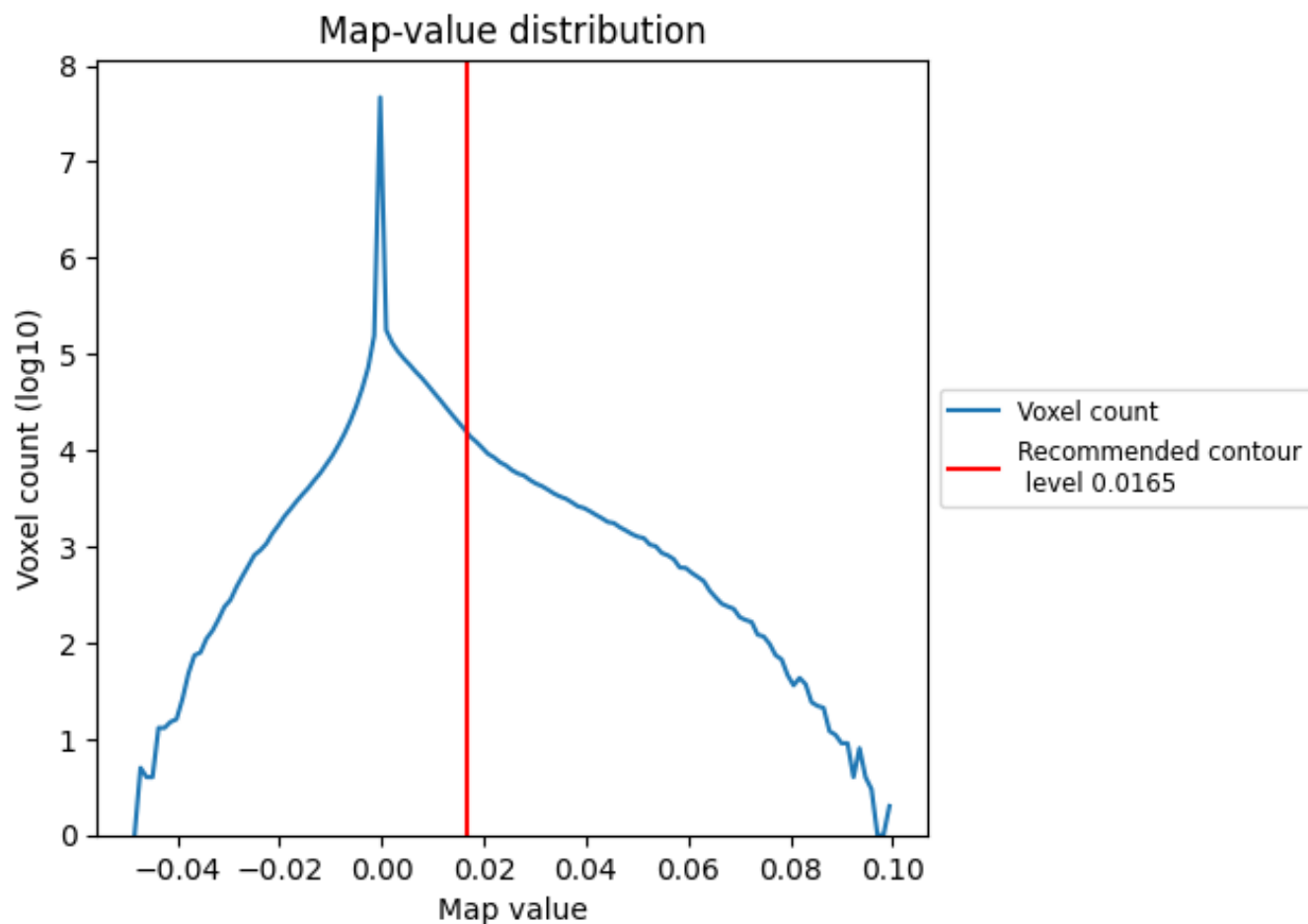


Z

7 Map analysis [i](#)

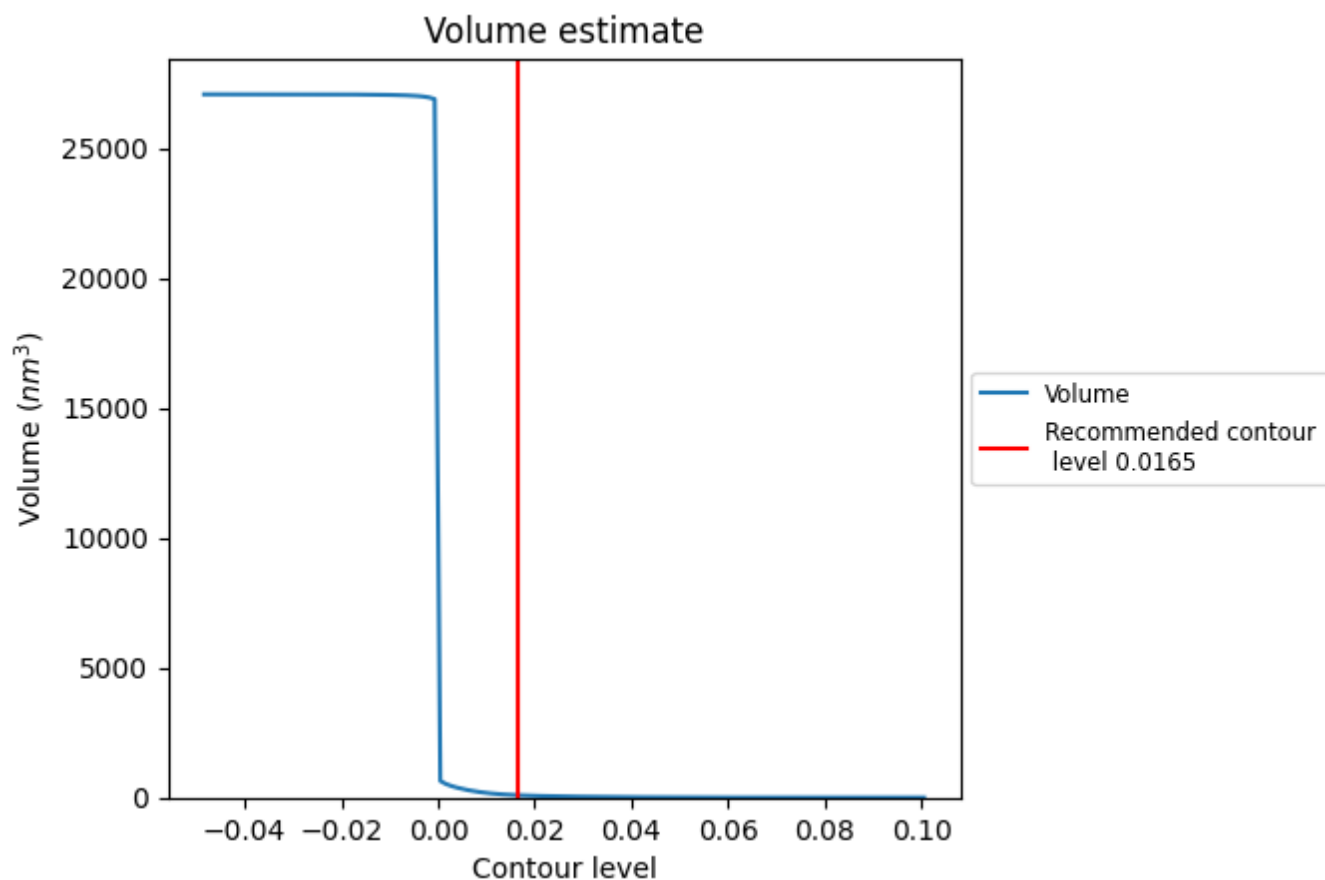
This section contains the results of statistical analysis of the map.

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.

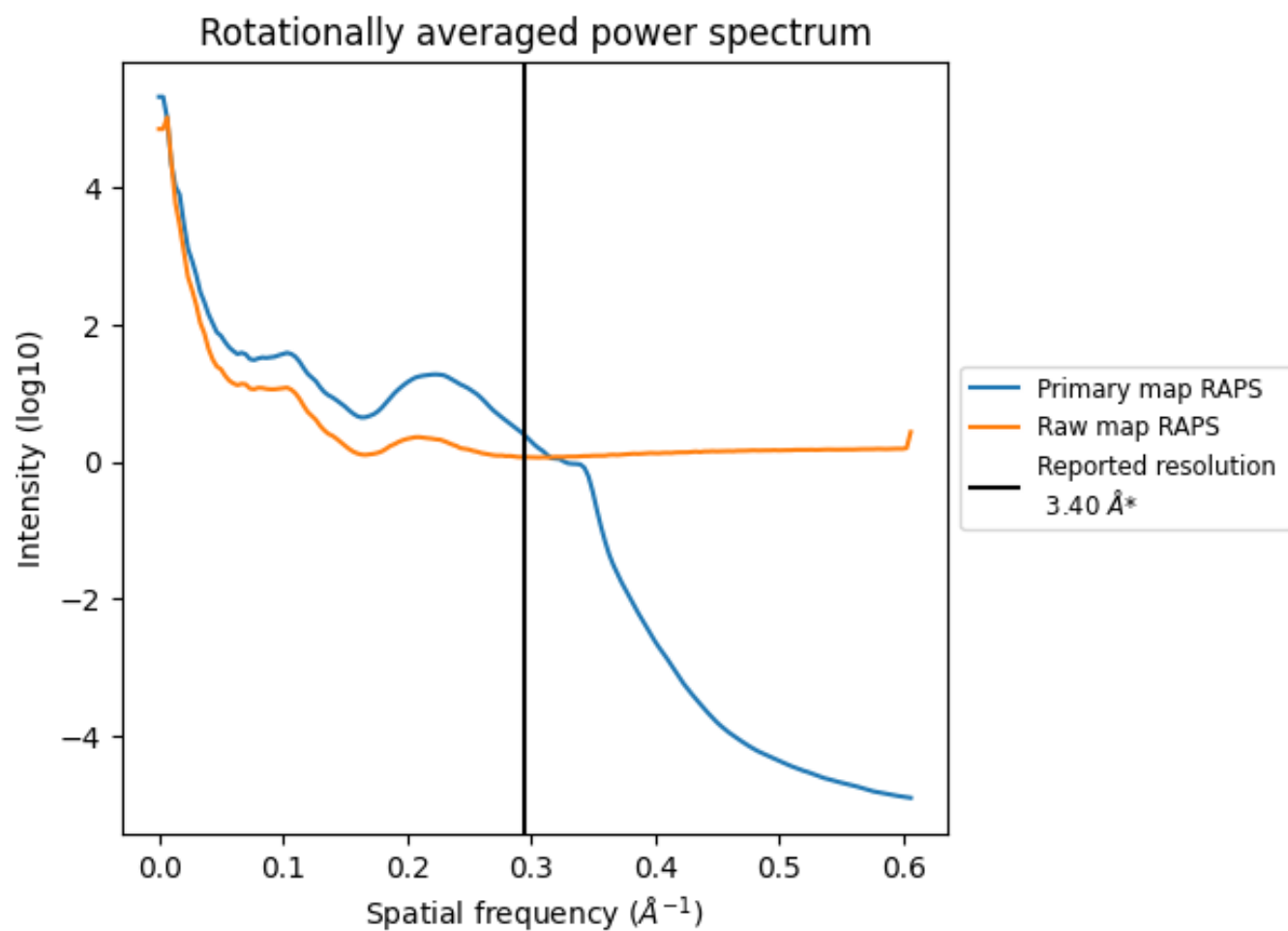
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 90 nm^3 ; this corresponds to an approximate mass of 81 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 ⓘ

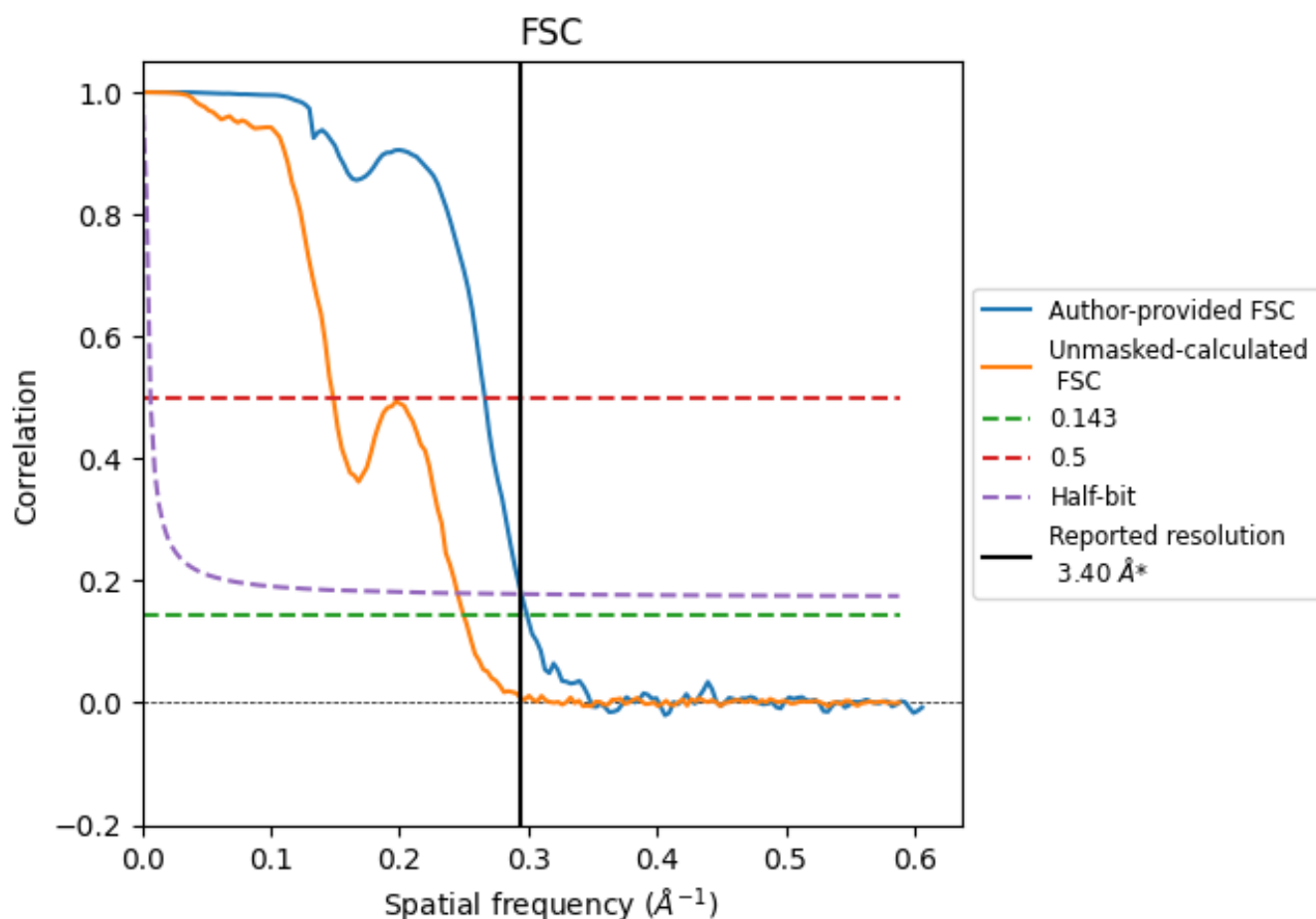


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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

8.2 Resolution estimates [i](#)

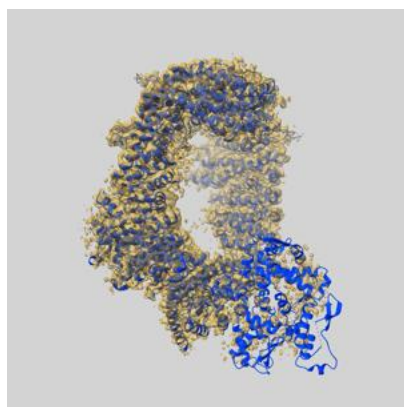
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.34	3.76	3.39
Unmasked-calculated*	4.00	6.74	4.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 3.4 by more than 10 %

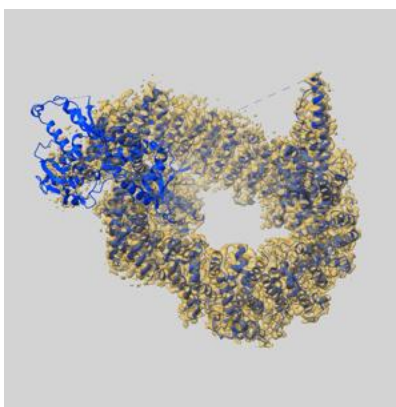
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22429 and PDB model 7MWE. Per-residue inclusion information can be found in section 3 on page 5.

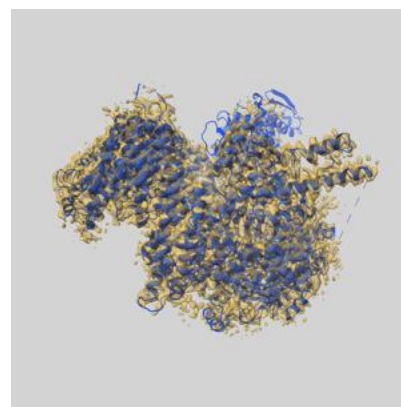
9.1 Map-model overlay [i](#)



X



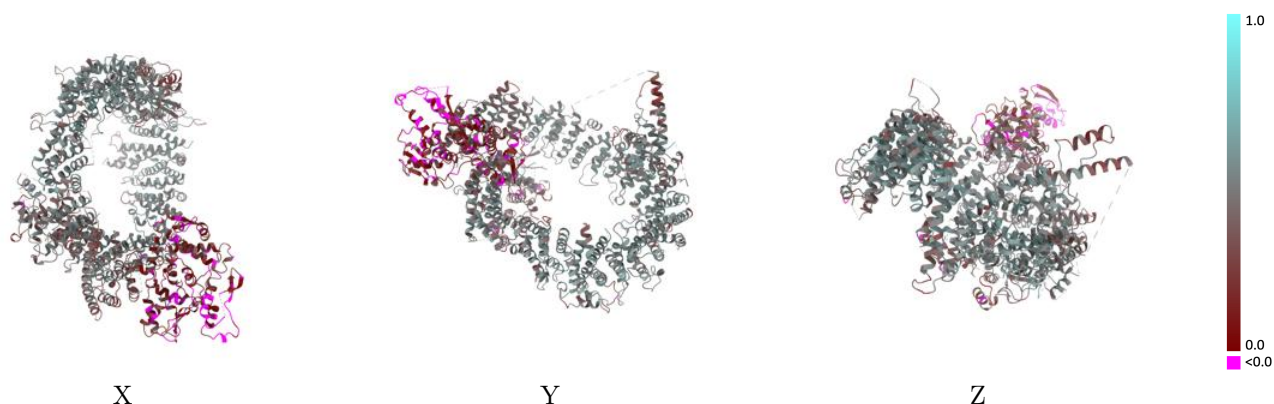
Y



Z

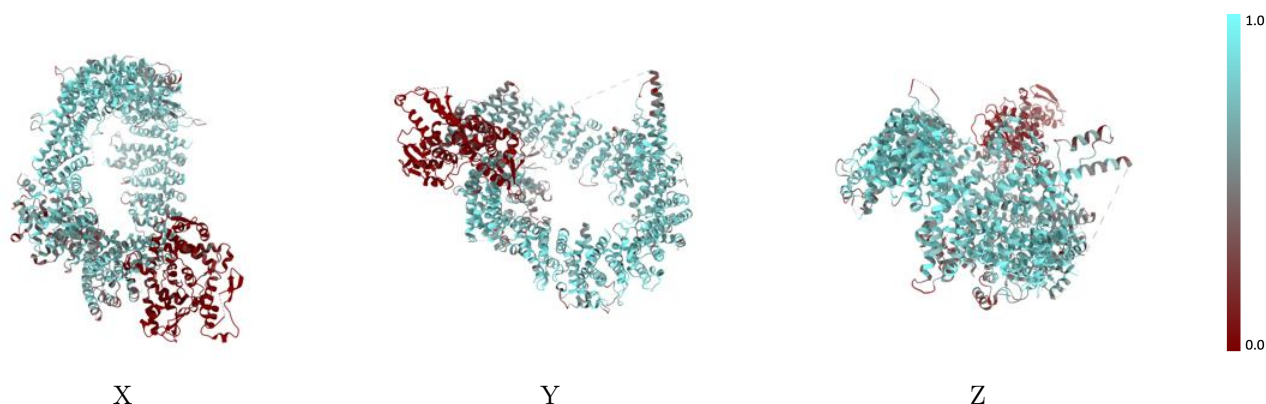
The images above show the 3D surface view of the map at the recommended contour level 0.0165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



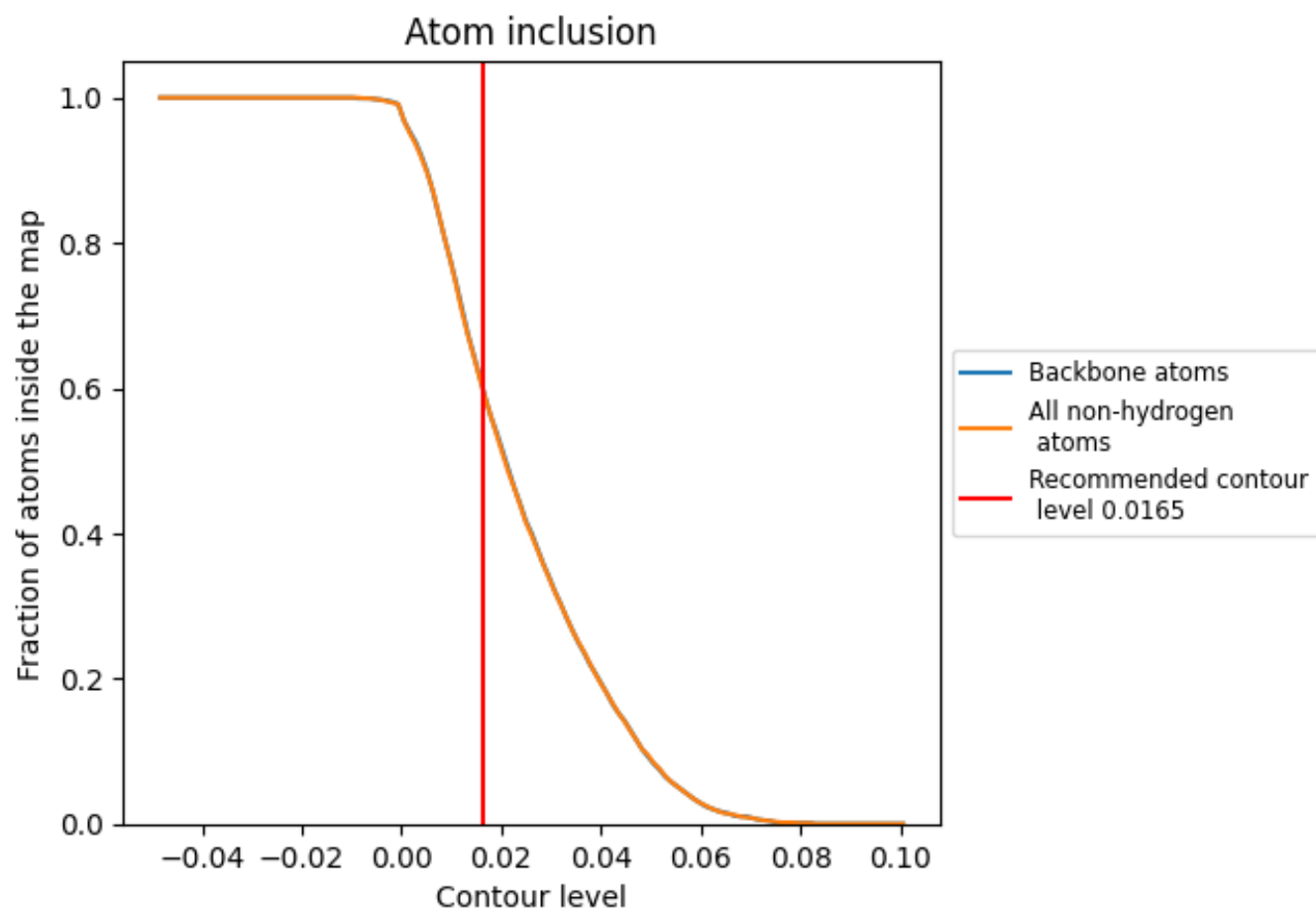
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0165).

9.4 Atom inclusion [i](#)



At the recommended contour level, 59% 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 (0.0165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5940	0.4090
A	0.5950	0.4090

