



wwPDB EM Validation Summary Report ⓘ

Jun 11, 2024 – 07:46 am BST

PDB ID : 8ORQ
EMDB ID : EMD-17130
Title : Cryo-EM structure of Pyrococcus furiosus apo form RNA polymerase open clamp conformation
Authors : Tarau, D.M.; Reichelt, R.; Heiss, F.B.; Pilsl, M.; Hausner, W.; Engel, C.; Grohmann, D.
Deposited on : 2023-04-17
Resolution : 3.20 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) : 2.36.2

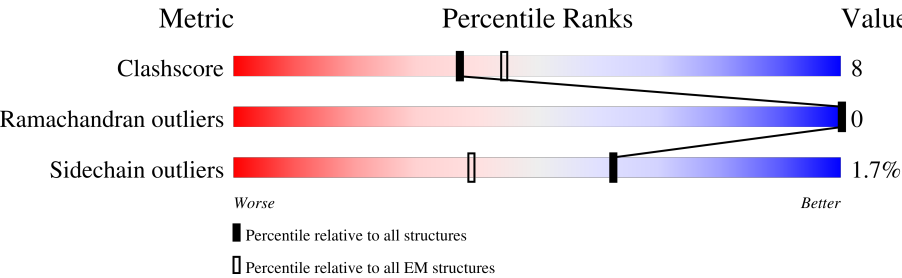
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	910	78% 20% ..
2	B	1117	80% 15% ..
3	C	397	70% 27% ..
4	D	275	86% 8% 6%
5	E	189	37% 61% 37% .
6	F	120	29% 51% 47% .
7	L	95	89% 9% .
8	H	82	73% 18% . 7%

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Mol	Chain	Length	Quality of chain
9	N	65	<div><div></div><div>85%</div><div>15%</div></div>
10	K	57	<div><div></div><div>91%</div><div><div></div><div></div><div></div></div></div>
11	P	49	<div><div></div><div>88%</div><div>10%<div></div></div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 26195 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 DNA-directed RNA polymerase subunit Rpo1N.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	901	Total	C	N	O	S	0	0
			7197	4541	1282	1335	39		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1076	Total	C	N	O	S	0	0
			8637	5474	1533	1596	34		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit Rpo1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	388	Total	C	N	O	S	0	0
			3041	1921	525	585	10		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit Rpo3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	258	Total	C	N	O	S	0	0
			2086	1358	330	396	2		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	262	TRP	-	expression tag	UNP Q8U0E4
D	263	SER	-	expression tag	UNP Q8U0E4
D	264	HIS	-	expression tag	UNP Q8U0E4
D	265	PRO	-	expression tag	UNP Q8U0E4
D	266	GLN	-	expression tag	UNP Q8U0E4
D	267	PHE	-	expression tag	UNP Q8U0E4
D	268	GLU	-	expression tag	UNP Q8U0E4
D	269	LYS	-	expression tag	UNP Q8U0E4
D	270	HIS	-	expression tag	UNP Q8U0E4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	271	HIS	-	expression tag	UNP Q8U0E4
D	272	HIS	-	expression tag	UNP Q8U0E4
D	273	HIS	-	expression tag	UNP Q8U0E4
D	274	HIS	-	expression tag	UNP Q8U0E4
D	275	HIS	-	expression tag	UNP Q8U0E4

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit Rpo7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1496	971	247	272	6		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit Rpo4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	120	Total	C	N	O	S	0	0
			986	627	163	189	7		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit Rpo11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	94	Total	C	N	O	S	0	0
			777	500	129	146	2		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit Rpo5.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	76	Total	C	N	O	0	0
			609	398	100	111		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit Rpo10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	65	Total	C	N	O	S	0	0
			543	345	94	97	7		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit Rpo6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	55	Total	C	N	O	S	0	0
			424	281	71	71	1		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit Rpo12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	48	Total	C	N	O	S	0	0
			393	251	75	63	4		

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Mg	0
			1	1	

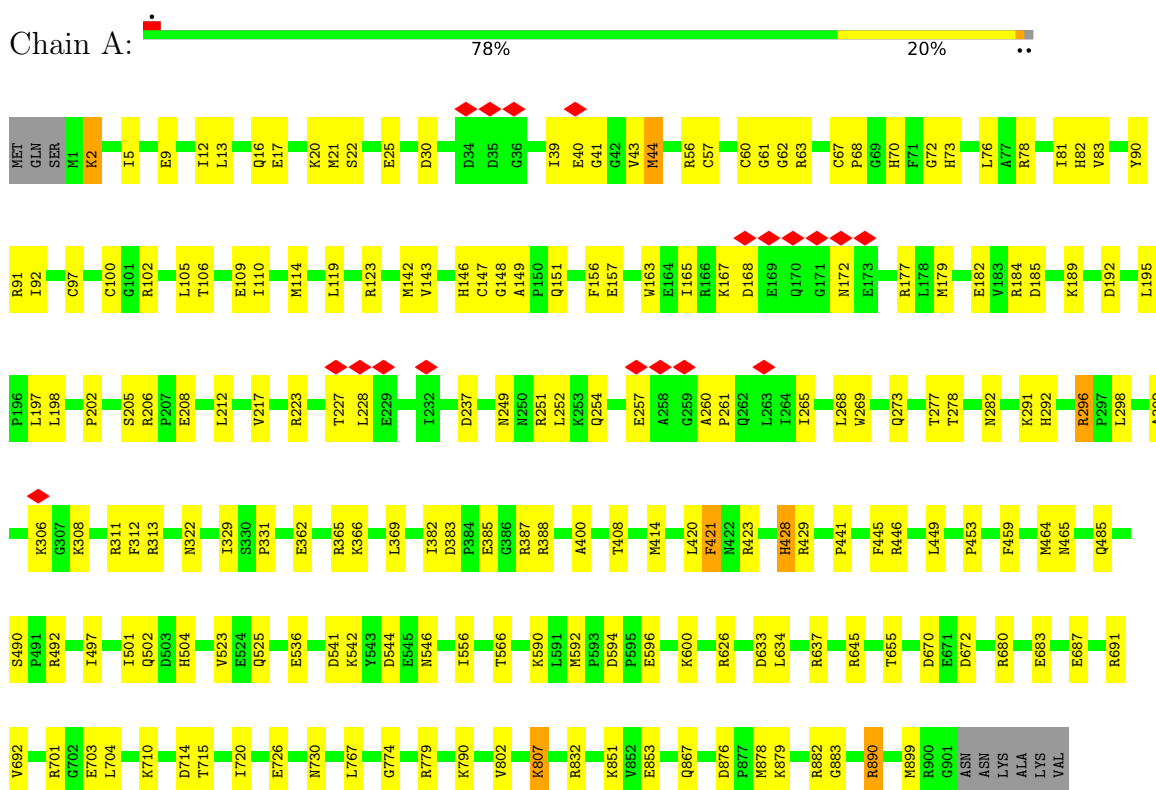
- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
13	A	2	Total	Zn	0
			2	2	
13	B	1	Total	Zn	0
			1	1	
13	N	1	Total	Zn	0
			1	1	
13	P	1	Total	Zn	0
			1	1	

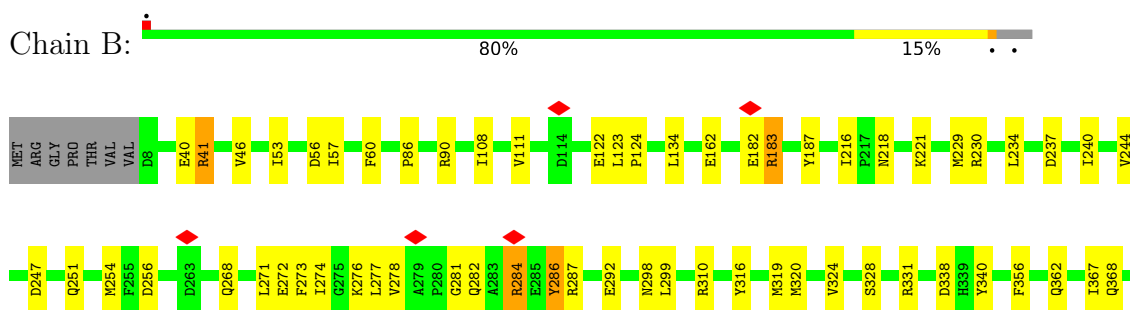
3 Residue-property plots

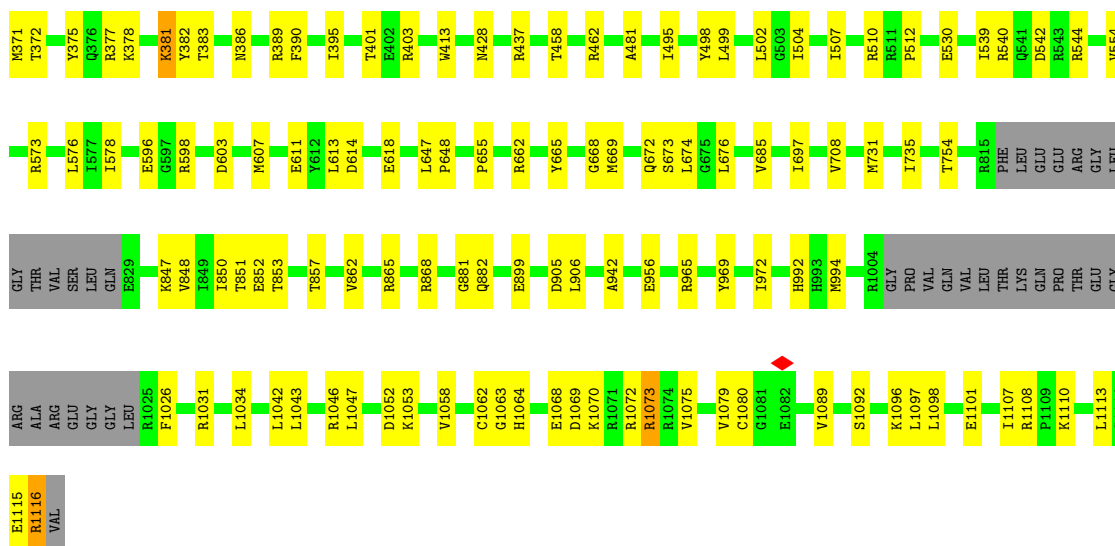
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-directed RNA polymerase subunit Rpo1N

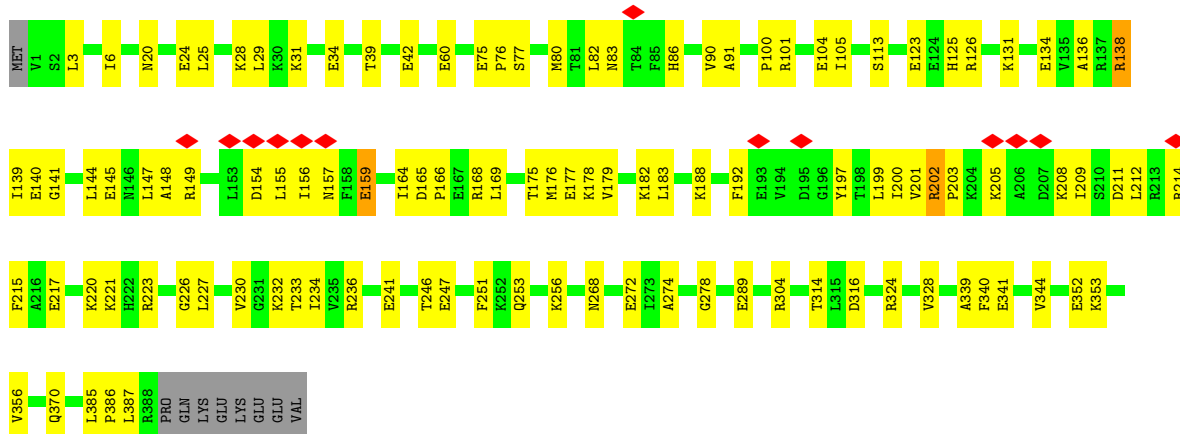


- Molecule 2: DNA-directed RNA polymerase subunit beta





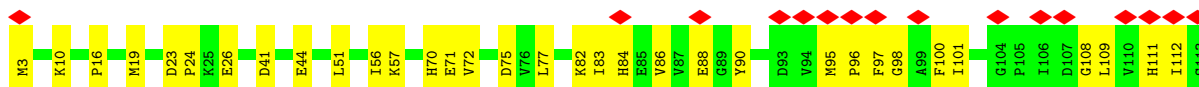
- Molecule 3: DNA-directed RNA polymerase subunit Rpo1C

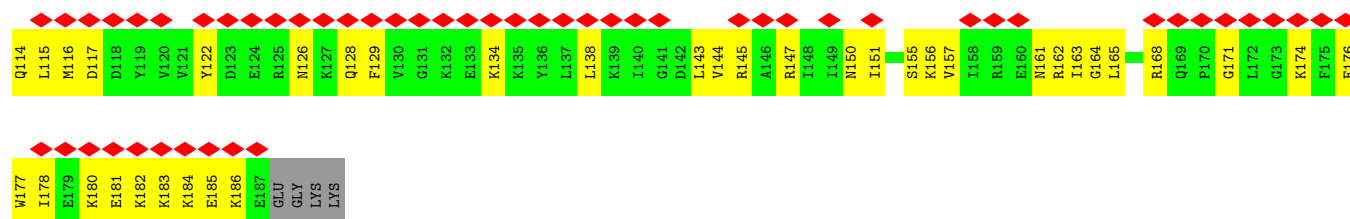


- Molecule 4: DNA-directed RNA polymerase subunit Rpo3



- Molecule 5: DNA-directed RNA polymerase subunit Rpo7

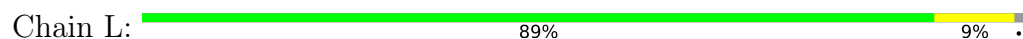




• Molecule 6: DNA-directed RNA polymerase subunit Rpo4



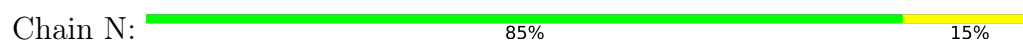
• Molecule 7: DNA-directed RNA polymerase subunit Rpo11



• Molecule 8: DNA-directed RNA polymerase subunit Rpo5



• Molecule 9: DNA-directed RNA polymerase subunit Rpo10



• Molecule 10: DNA-directed RNA polymerase subunit Rpo6



• Molecule 11: DNA-directed RNA polymerase subunit Rpo12





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161531	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.029	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	251.68, 251.68, 251.68	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.968, 0.968, 0.968	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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	0.30	0/7338	0.51	0/9907
2	B	0.31	0/8811	0.52	1/11905 (0.0%)
3	C	0.27	0/3081	0.49	0/4156
4	D	0.33	0/2133	0.45	0/2894
5	E	0.26	0/1524	0.53	0/2052
6	F	0.26	0/1000	0.54	0/1338
7	L	0.31	0/792	0.46	0/1067
8	H	0.33	0/622	0.47	0/841
9	N	0.36	0/553	0.53	0/740
10	K	0.31	0/433	0.53	0/588
11	P	0.30	0/400	0.60	0/534
All	All	0.30	0/26687	0.51	1/36022 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	905	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7197	0	7263	125	0
2	B	8637	0	8707	112	0
3	C	3041	0	3151	80	0
4	D	2086	0	2109	15	0
5	E	1496	0	1555	62	0
6	F	986	0	1001	56	0
7	L	777	0	788	8	0
8	H	609	0	634	9	0
9	N	543	0	541	6	0
10	K	424	0	460	3	0
11	P	393	0	423	2	0
12	A	1	0	0	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	N	1	0	0	0	0
13	P	1	0	0	0	0
All	All	26195	0	26632	432	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 8.

The worst 5 of 432 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)
6:F:93:ARG:NH2	6:F:108:MET:HG2	1.90	0.86
1:A:710:LYS:HB3	1:A:714:ASP:HB3	1.59	0.83
1:A:634:LEU:HD11	1:A:890:ARG:HE	1.48	0.79
6:F:108:MET:HA	6:F:111:ILE:HD12	1.64	0.79
7:L:22:HIS:HD1	7:L:43:TYR:HH	1.29	0.78

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	899/910 (99%)	856 (95%)	43 (5%)	0	100	100
2	B	1070/1117 (96%)	1033 (96%)	37 (4%)	0	100	100
3	C	386/397 (97%)	376 (97%)	10 (3%)	0	100	100
4	D	256/275 (93%)	254 (99%)	2 (1%)	0	100	100
5	E	183/189 (97%)	177 (97%)	6 (3%)	0	100	100
6	F	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
7	L	92/95 (97%)	88 (96%)	4 (4%)	0	100	100
8	H	74/82 (90%)	74 (100%)	0	0	100	100
9	N	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
10	K	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
11	P	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
All	All	3240/3356 (96%)	3127 (96%)	113 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	777/785 (99%)	763 (98%)	14 (2%)	59	82
2	B	929/962 (97%)	916 (99%)	13 (1%)	67	86
3	C	336/345 (97%)	330 (98%)	6 (2%)	59	82
4	D	230/246 (94%)	230 (100%)	0	100	100
5	E	164/167 (98%)	162 (99%)	2 (1%)	71	88
6	F	103/103 (100%)	99 (96%)	4 (4%)	32	67
7	L	83/84 (99%)	82 (99%)	1 (1%)	71	88
8	H	66/70 (94%)	62 (94%)	4 (6%)	18	54
9	N	60/60 (100%)	59 (98%)	1 (2%)	60	83
10	K	45/47 (96%)	44 (98%)	1 (2%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	P	44/45 (98%)	42 (96%)	2 (4%)	27 63
All	All	2837/2914 (97%)	2789 (98%)	48 (2%)	62 83

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	159	GLU
6	F	25	ARG
3	C	202	ARG
3	C	221	LYS
6	F	73	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
2	B	218	ASN
3	C	253	GLN
3	C	370	GLN
5	E	126	ASN

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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

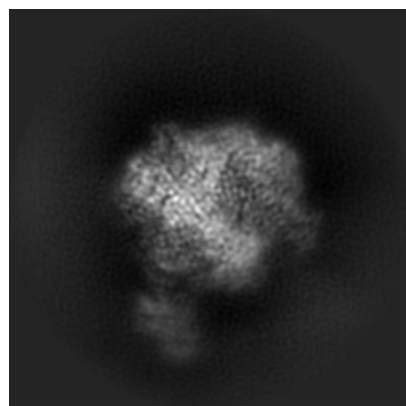
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17130. These allow visual inspection of the internal detail of the map and identification of artifacts.

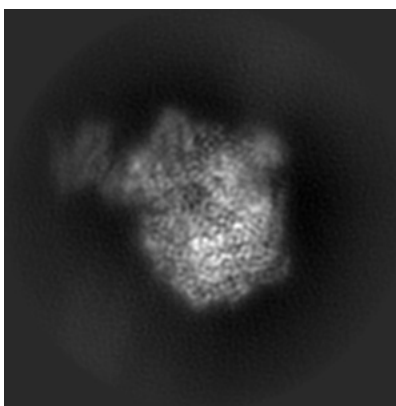
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

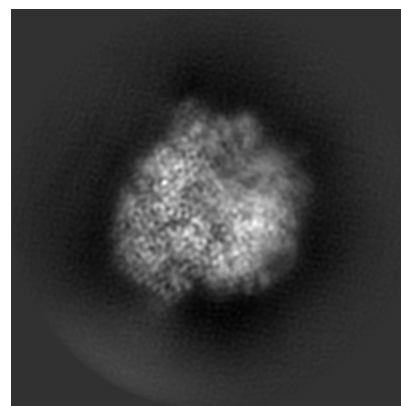
6.1.1 Primary map



X

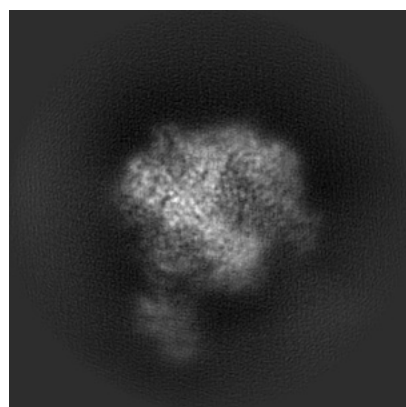


Y

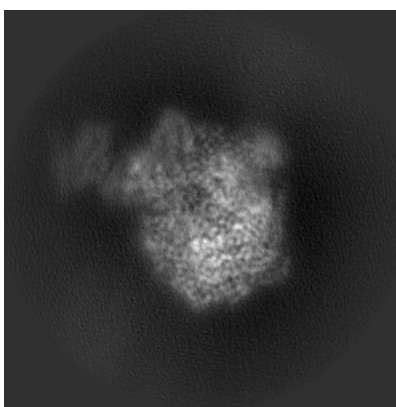


Z

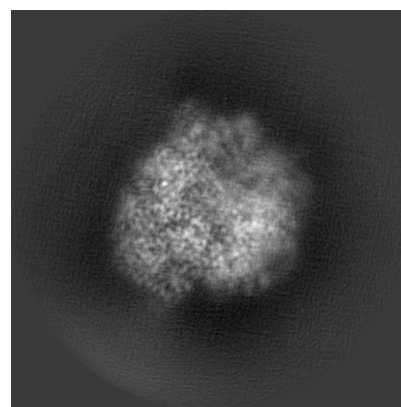
6.1.2 Raw map



X



Y

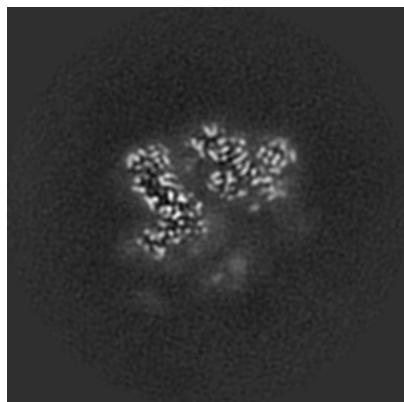


Z

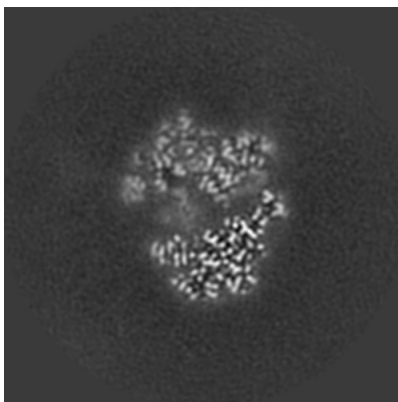
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

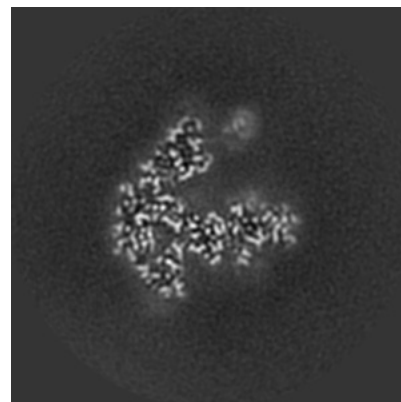
6.2.1 Primary map



X Index: 130

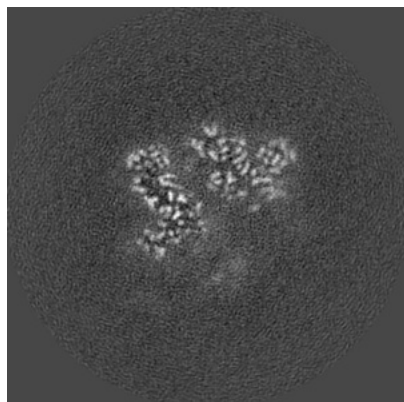


Y Index: 130

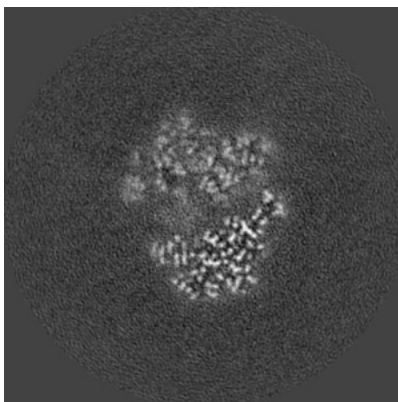


Z Index: 130

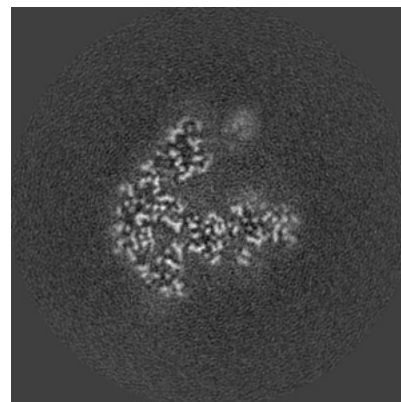
6.2.2 Raw map



X Index: 130



Y Index: 130

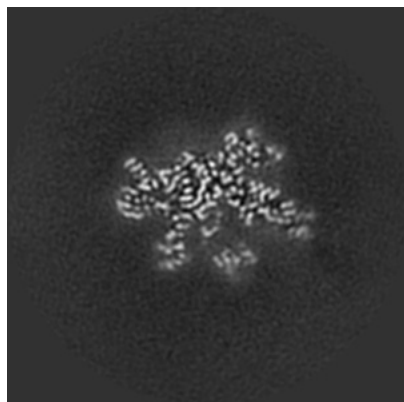


Z Index: 130

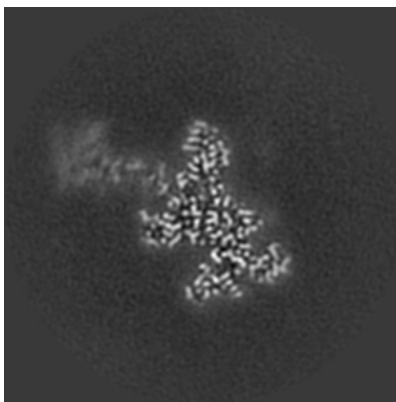
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

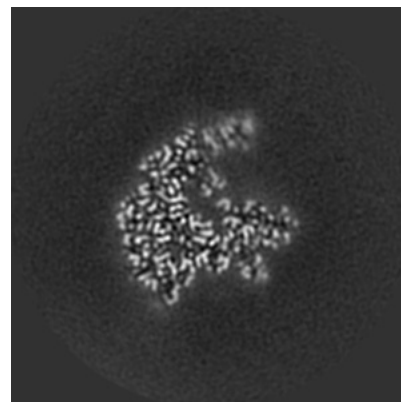
6.3.1 Primary map



X Index: 109

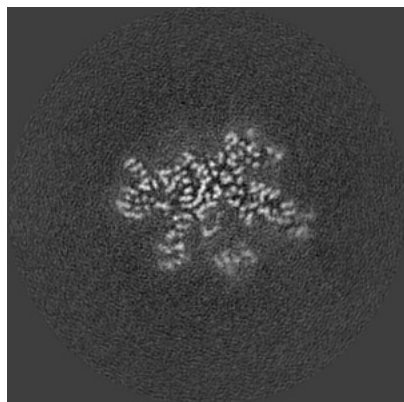


Y Index: 108

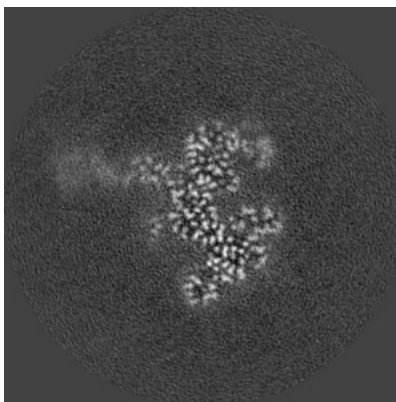


Z Index: 137

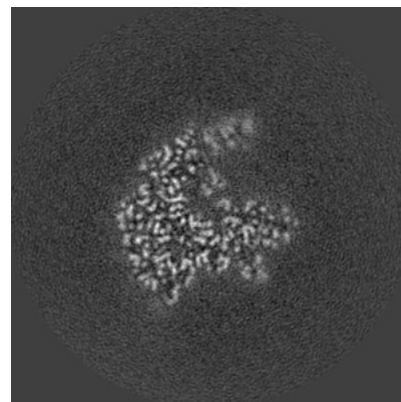
6.3.2 Raw map



X Index: 109



Y Index: 117

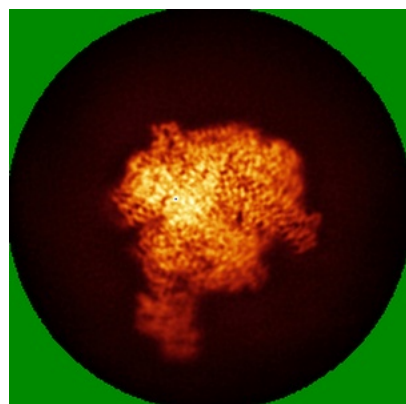


Z Index: 137

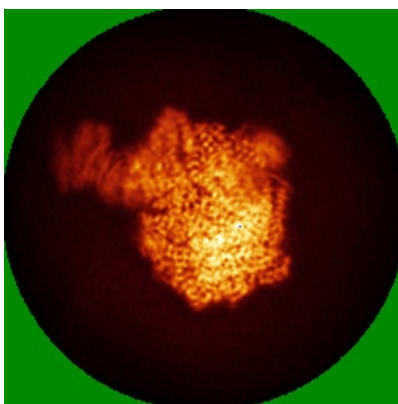
The images above show the largest variance slices of the map in three orthogonal directions.

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

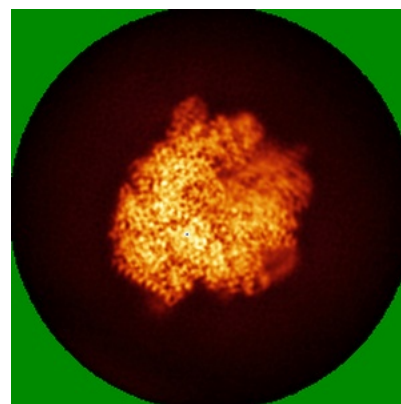
6.4.1 Primary map



X

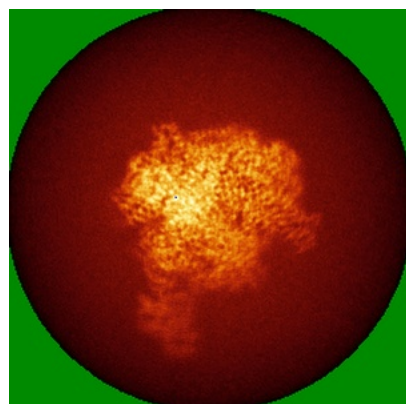


Y

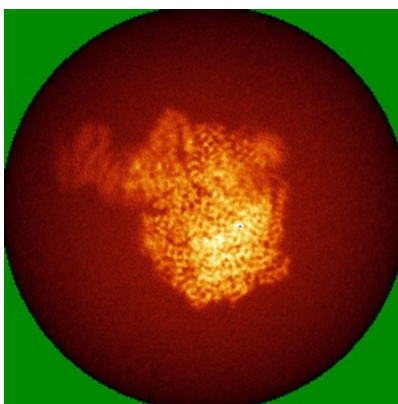


Z

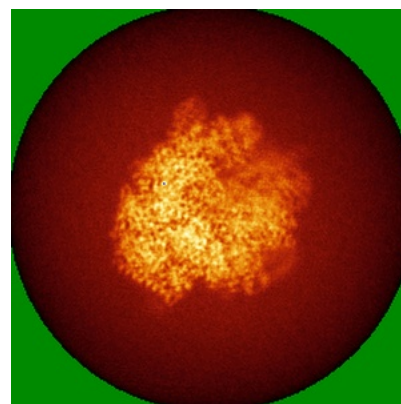
6.4.2 Raw map



X



Y

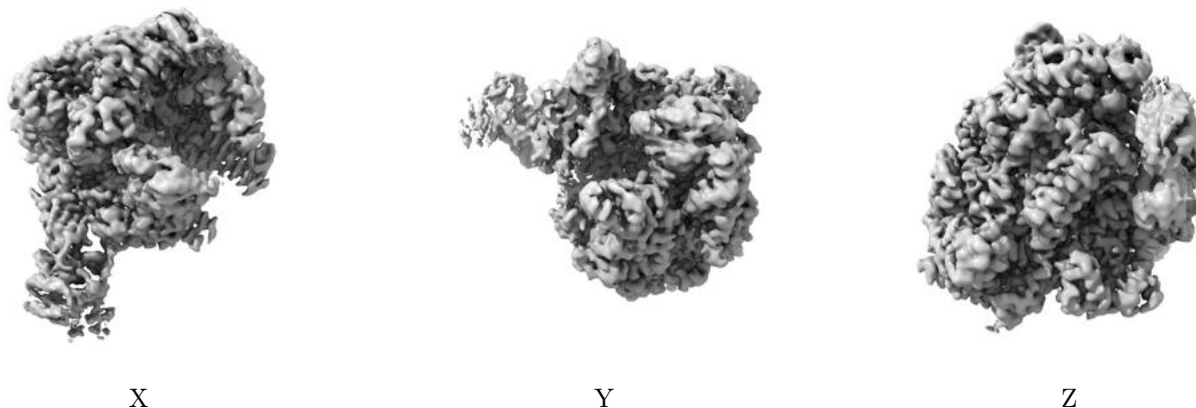


Z

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.

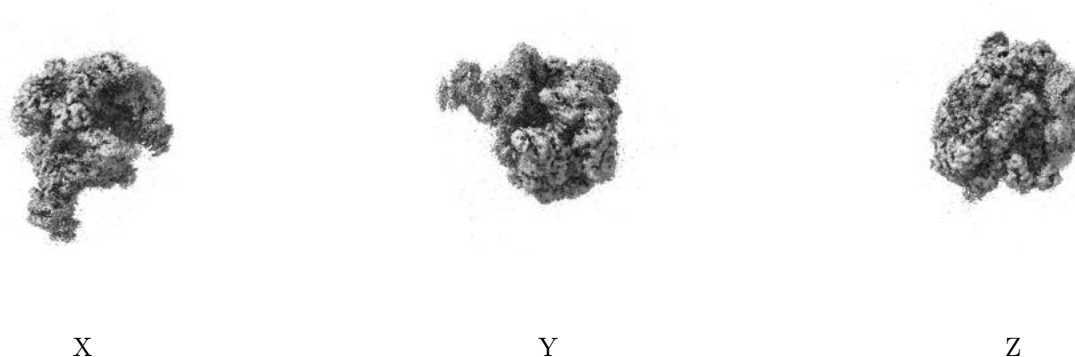
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

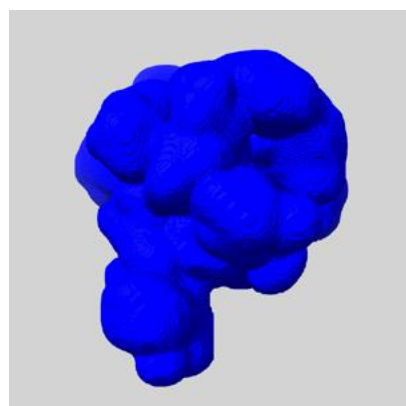
6.6 Mask visualisation [i](#)

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

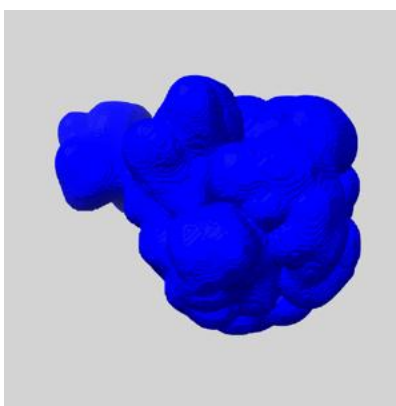
A mask typically either:

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

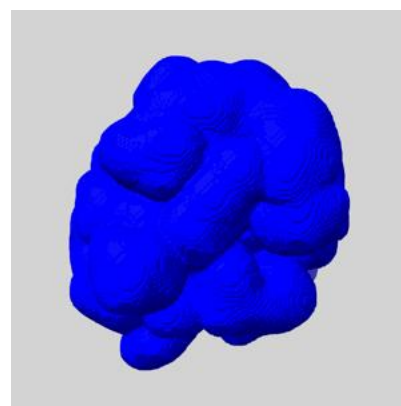
6.6.1 emd_17130_msk_1.map [i](#)



X



Y

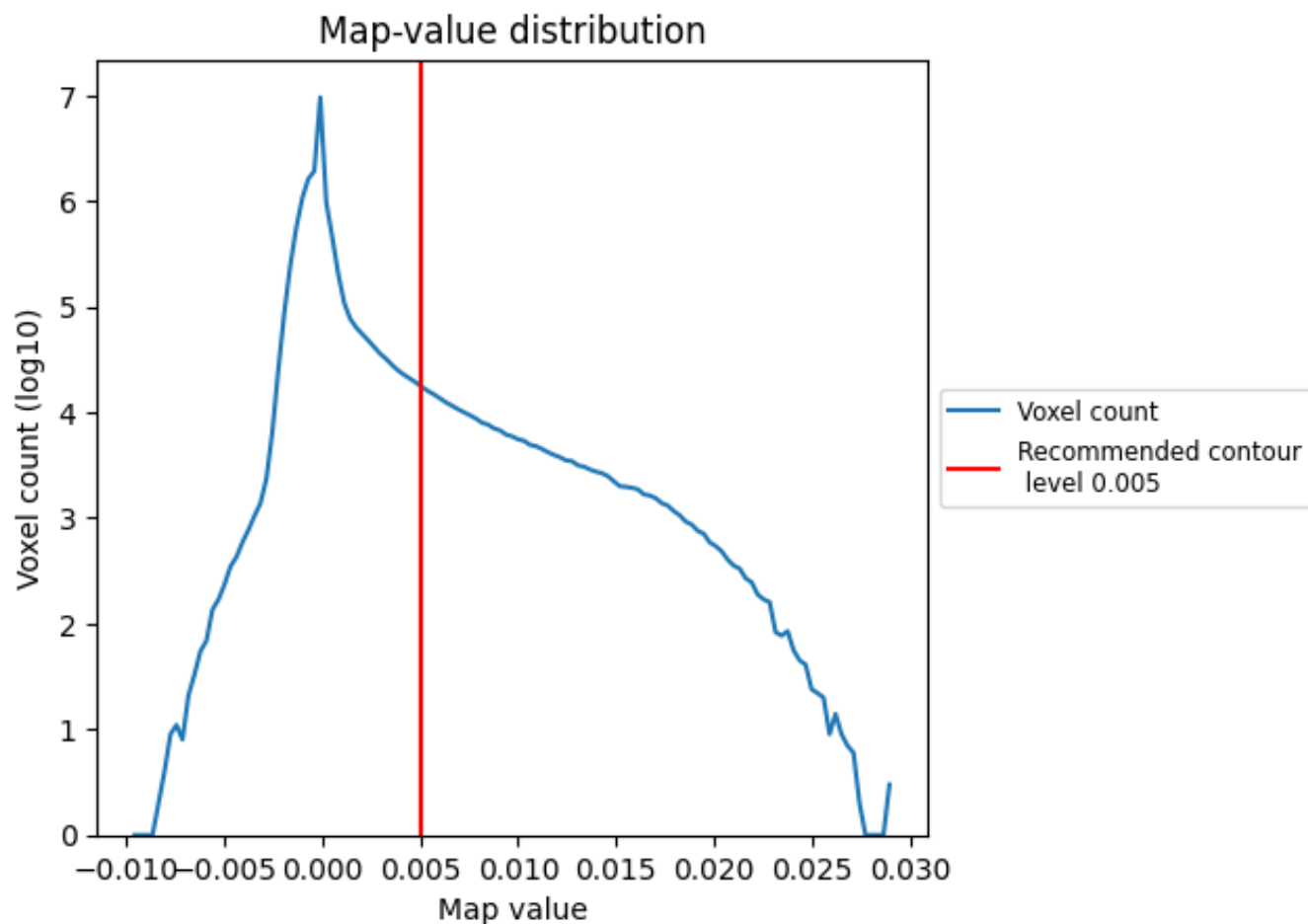


Z

7 Map analysis [i](#)

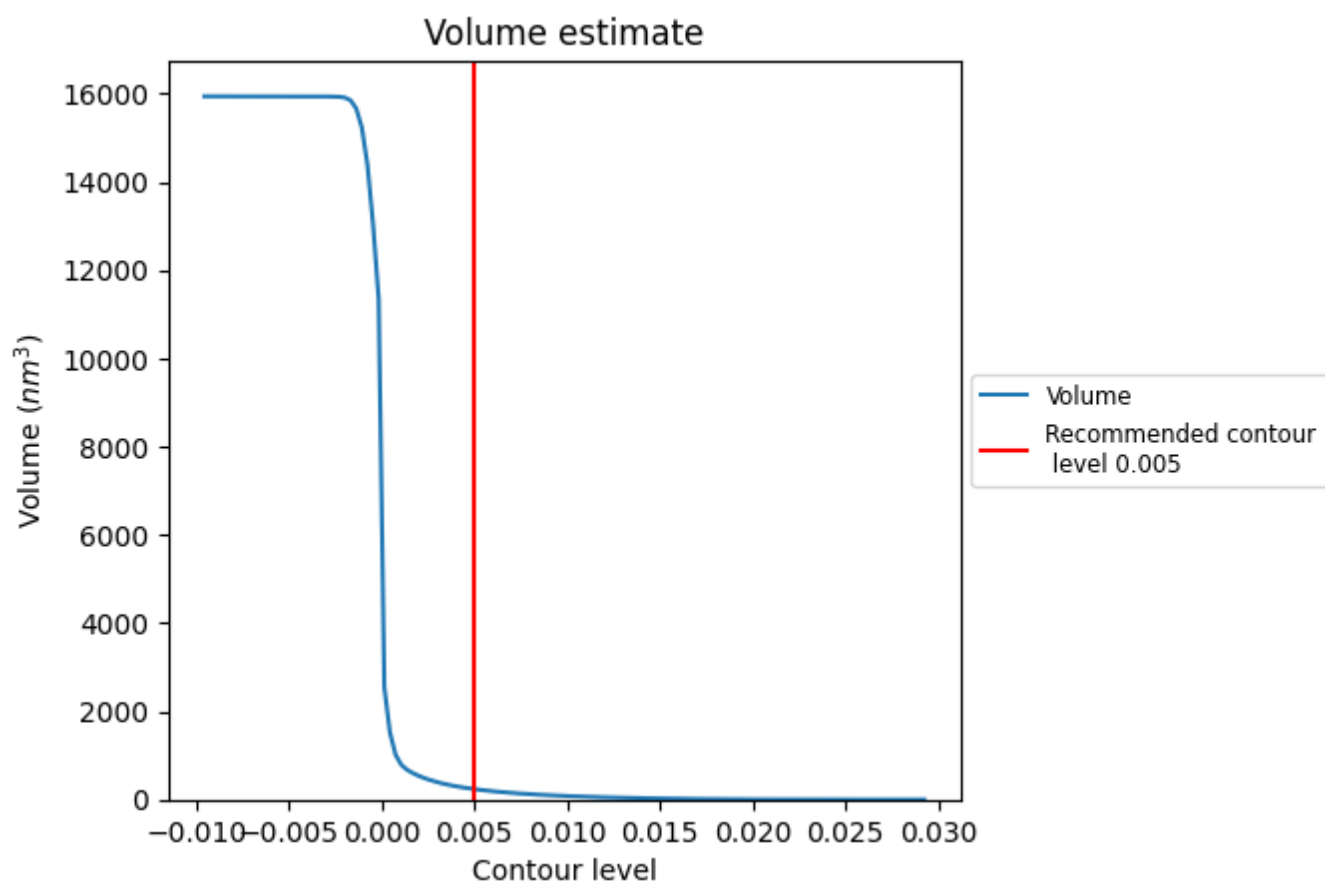
This section contains the results of statistical analysis of the map.

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.

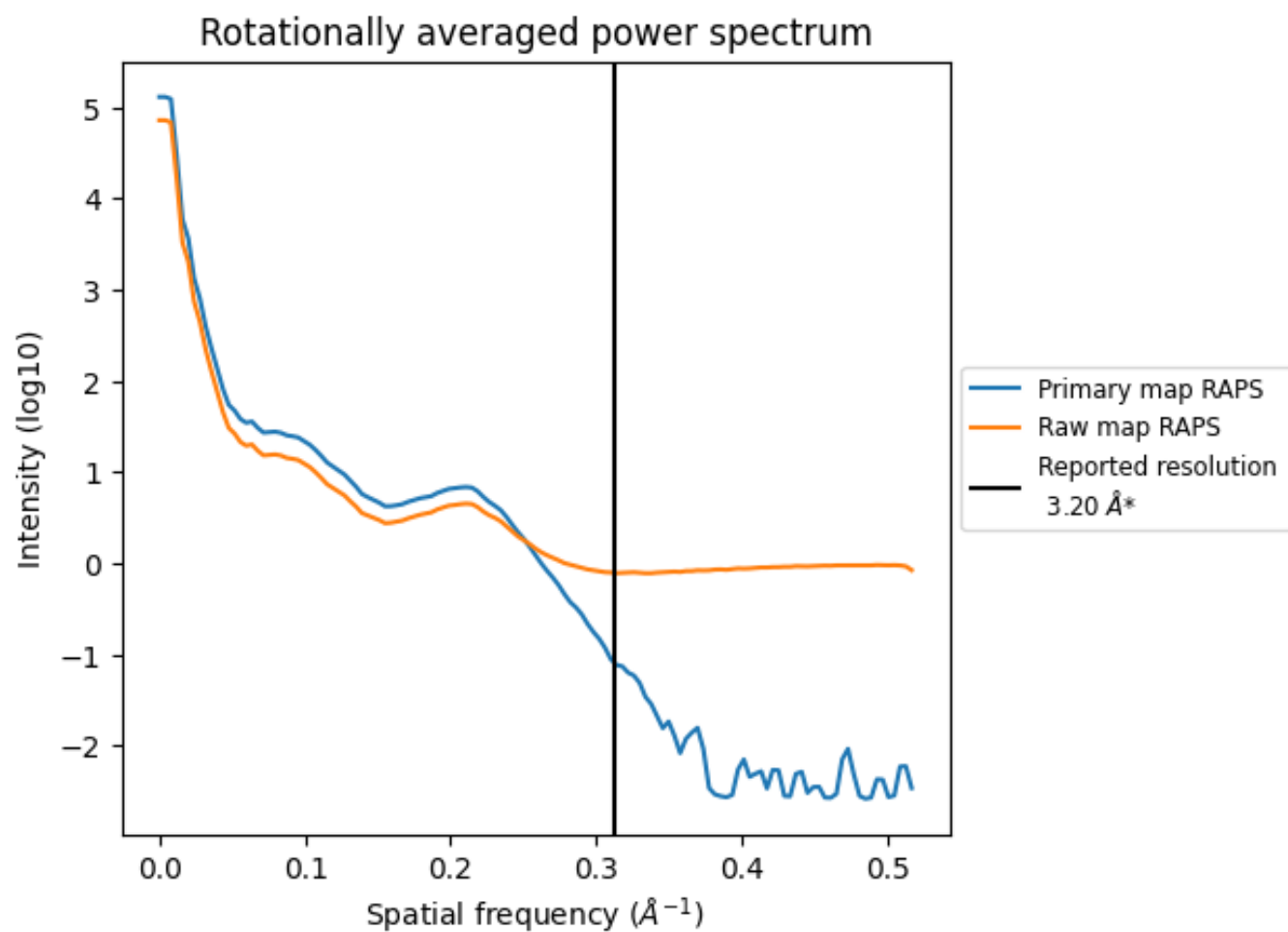
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 236 nm³; this corresponds to an approximate mass of 213 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 ⓘ

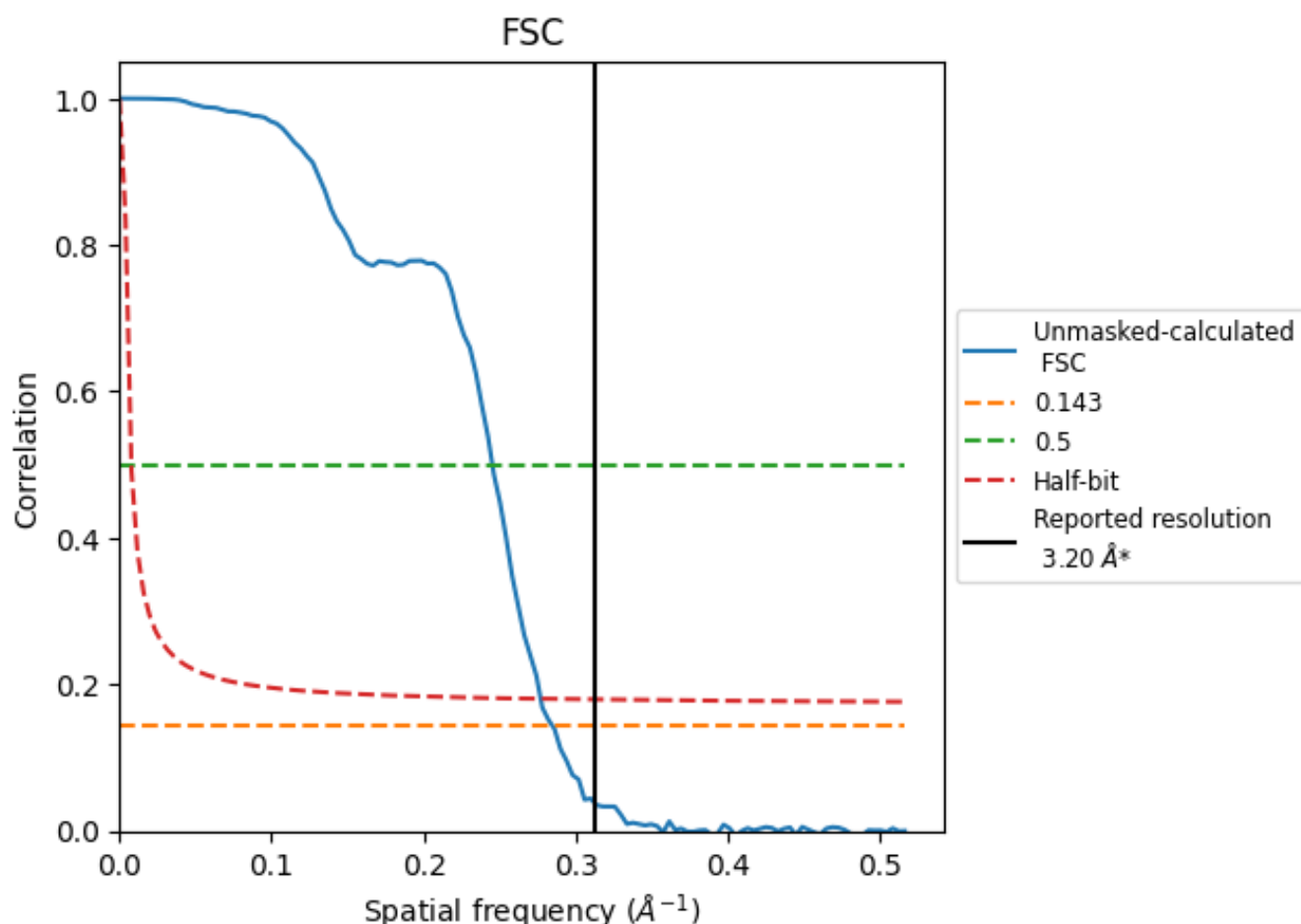


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

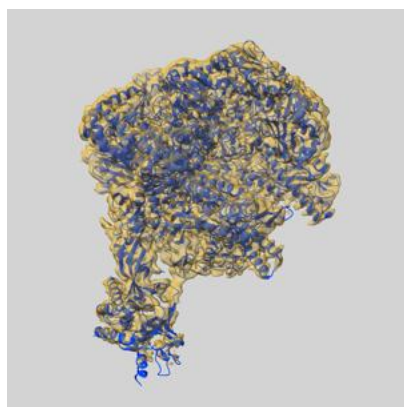
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	4.08	3.61

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

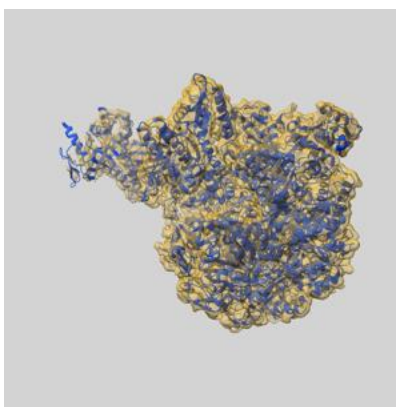
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17130 and PDB model 8ORQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

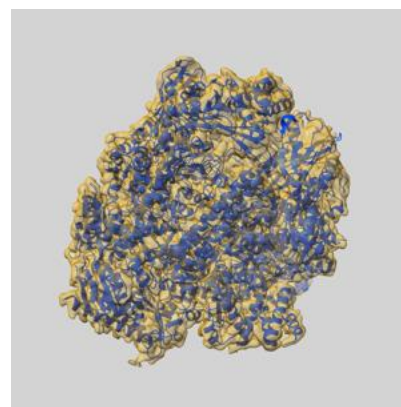
9.1 Map-model overlay [i](#)



X



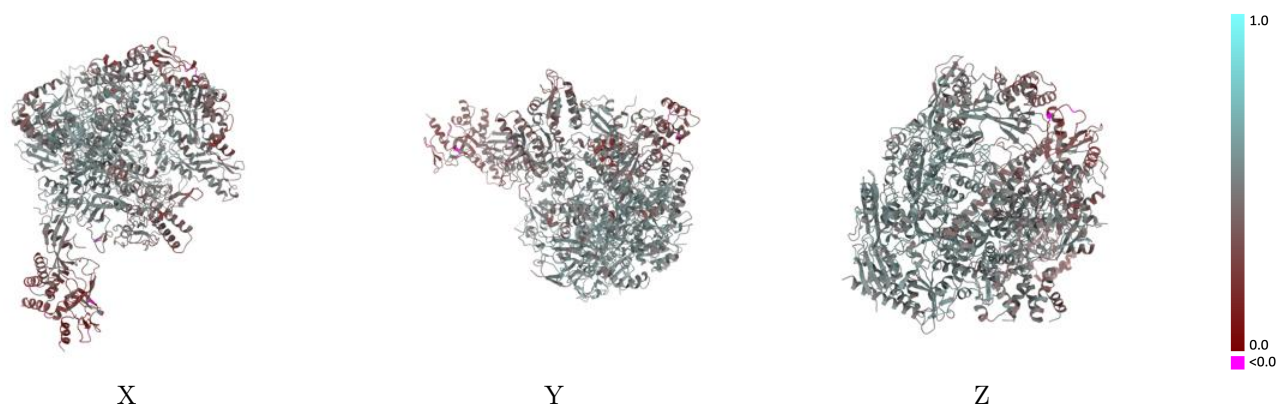
Y



Z

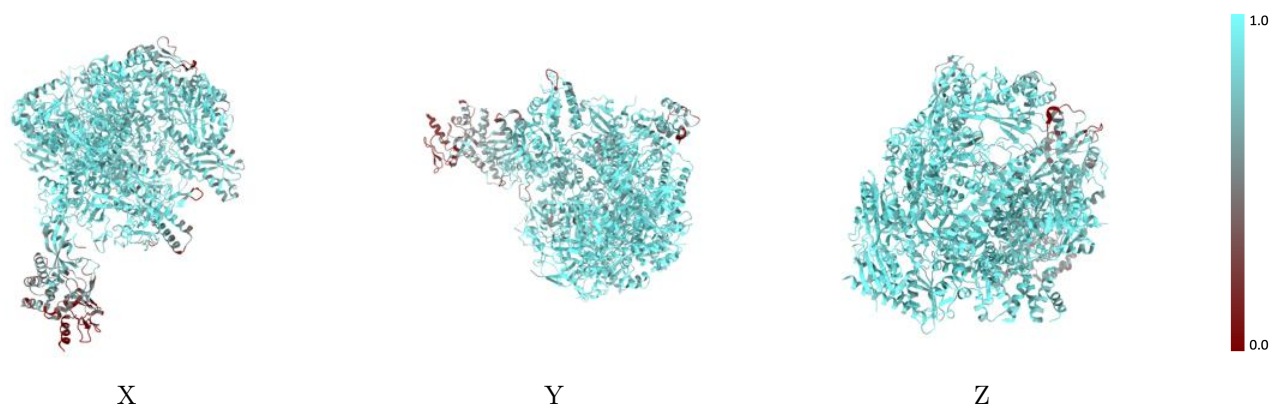
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



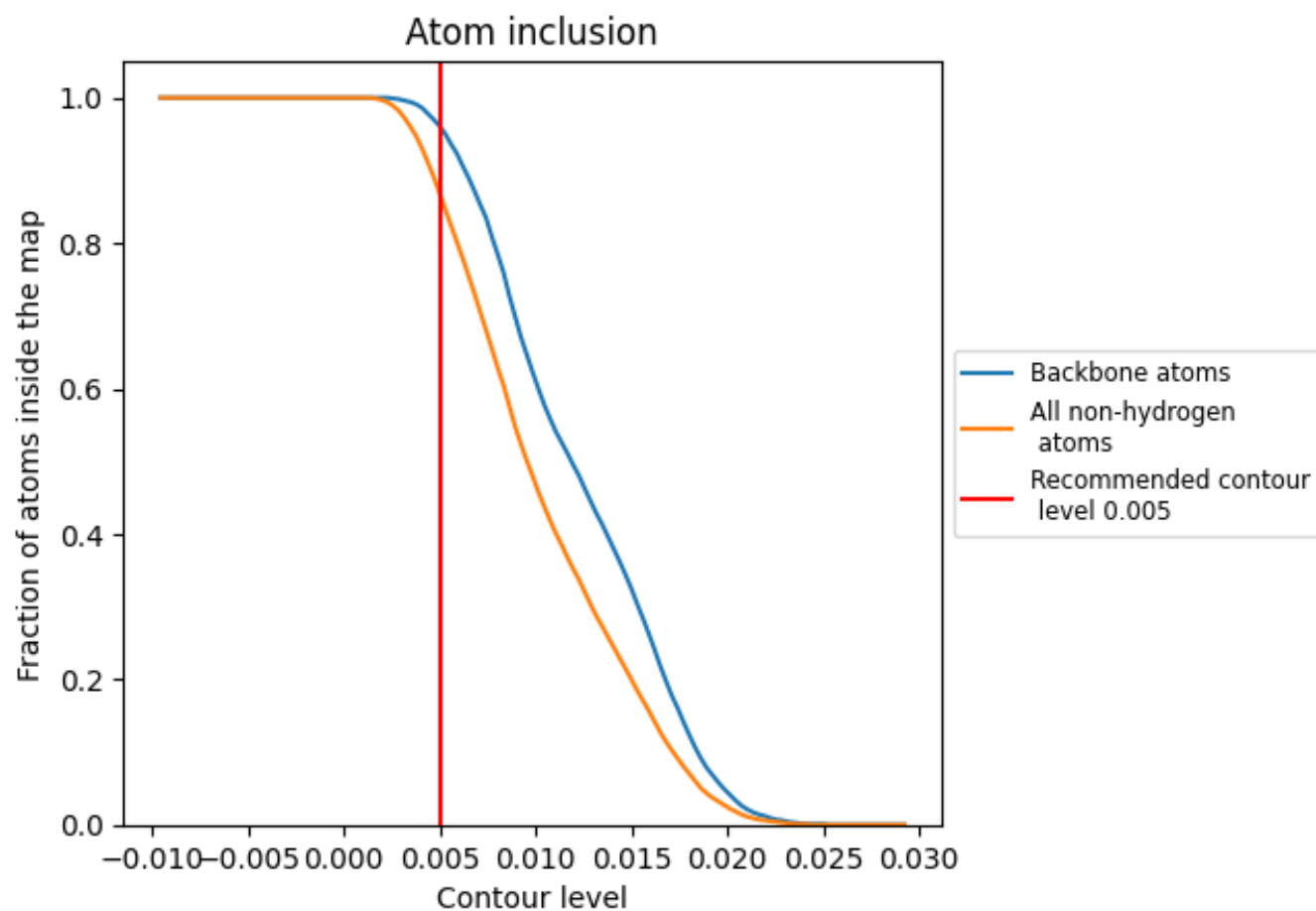
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 87% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8680	<div></div> 0.4770
A	<div></div> 0.9000	<div></div> 0.4840
B	<div></div> 0.9210	<div></div> 0.5050
C	<div></div> 0.8260	<div></div> 0.4320
D	<div></div> 0.9440	<div></div> 0.5300
E	<div></div> 0.5040	<div></div> 0.3310
F	<div></div> 0.5230	<div></div> 0.3010
H	<div></div> 0.9280	<div></div> 0.5130
K	<div></div> 0.9520	<div></div> 0.5170
L	<div></div> 0.9250	<div></div> 0.5290
N	<div></div> 0.9640	<div></div> 0.5390
P	<div></div> 0.9100	<div></div> 0.5120

1.0

0.0

<0.0