



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 03:29 PM JST

PDB ID : 6M6A
EMDB ID : EMD-30117
Title : Cryo-EM structure of *Thermus thermophilus* Mfd in complex with RNA polymerase
Authors : Shi, J.; Wen, A.; Feng, Y.
Deposited on : 2020-03-14
Resolution : 5.00 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

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

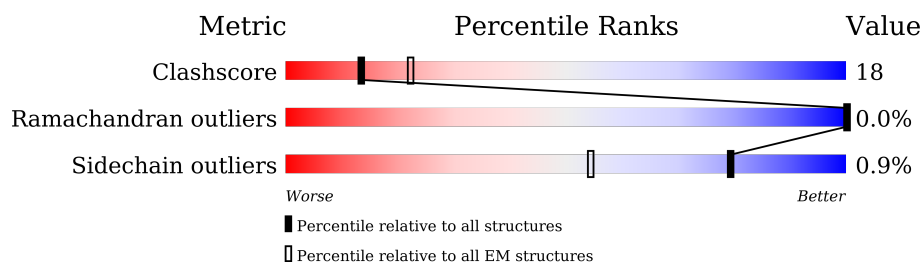
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 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	315	 41% 30% 28%
1	B	315	 42% 28% 30%
2	C	1119	 64% 35%
3	D	1524	 53% 32% 14%
4	E	99	 67% 27% 5%
5	M	978	 27% 20% 53%
6	T	63	 24% 21% 56%
7	N	63	 21% 24% 56%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 28142 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1782	1138	310	332	2		
1	B	222	Total	C	N	O	S	0	0
			1750	1118	304	326	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8770	5548	1564	1634	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1304	Total	C	N	O	S	0	0
			10293	6515	1825	1921	32		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	94	Total	C	N	O	S	0	0
			761	486	132	139	4		

- Molecule 5 is a protein called Transcription-repair-coupling factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	459	Total	C	N	O	S	0	0
			3635	2327	645	659	4		

- Molecule 6 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	28	Total	C	N	O	P	0	0
			574	272	106	168	28		

- Molecule 7 is a DNA chain called nontemplate strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	28	Total	C	N	O	P	0	0
			574	272	106	168	28		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	D	2	Total	Zn	0
			2	2	

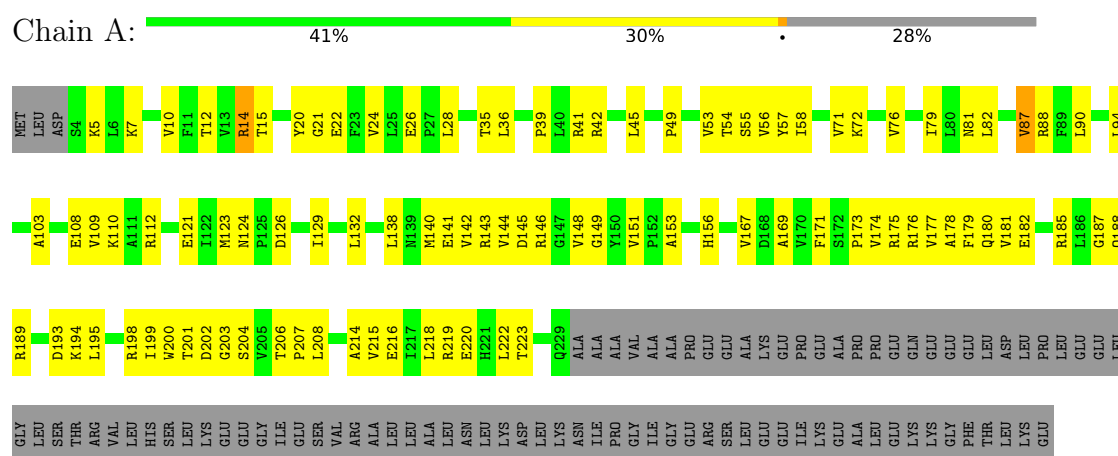
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total	Mg	0
			1	1	

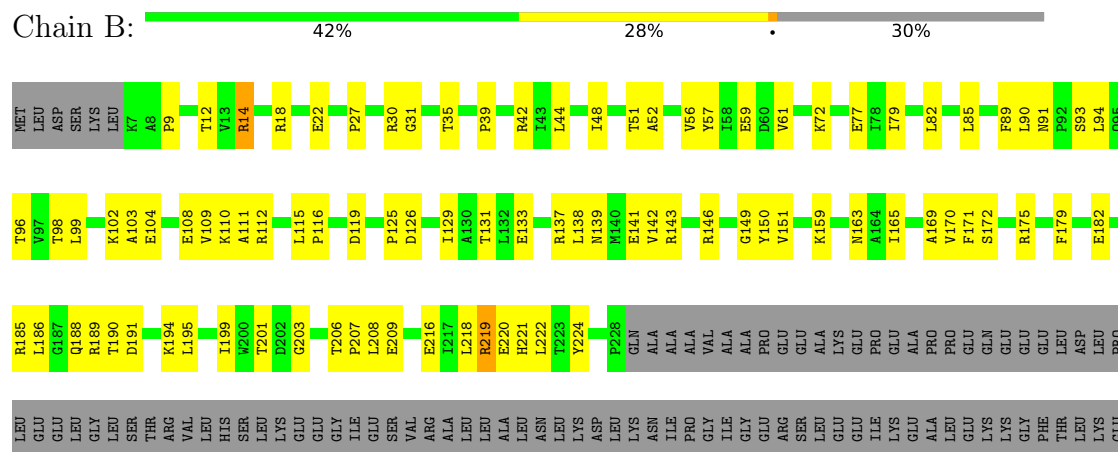
3 Residue-property plots

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 alpha

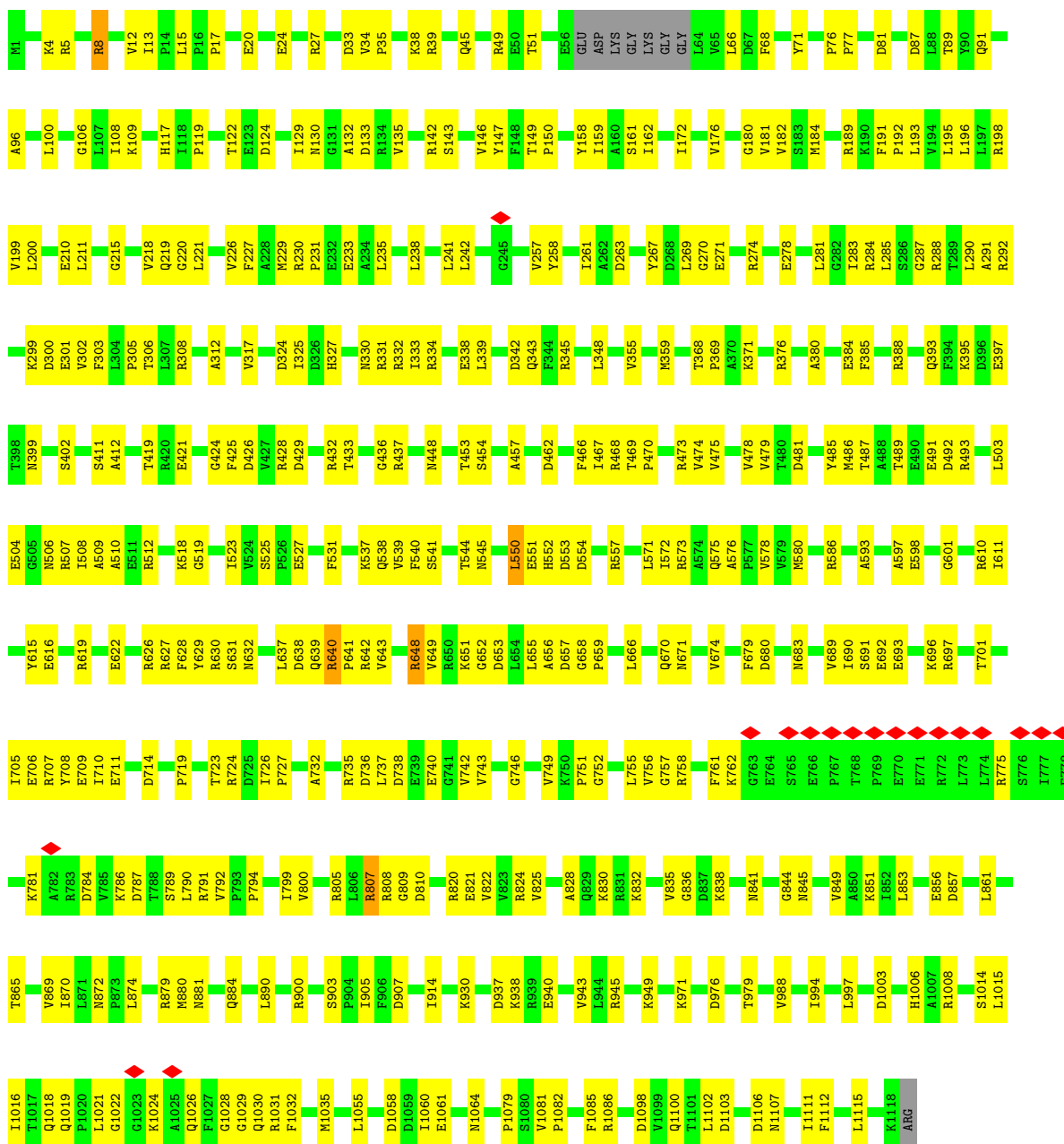


• Molecule 1: DNA-directed RNA polymerase subunit alpha



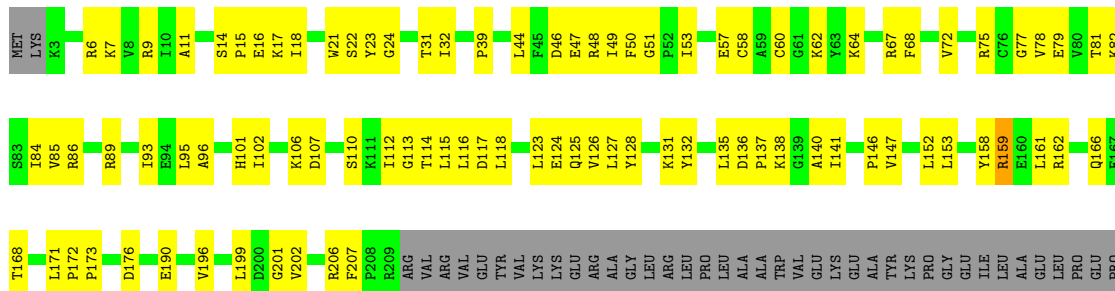
• Molecule 2: DNA-directed RNA polymerase subunit beta





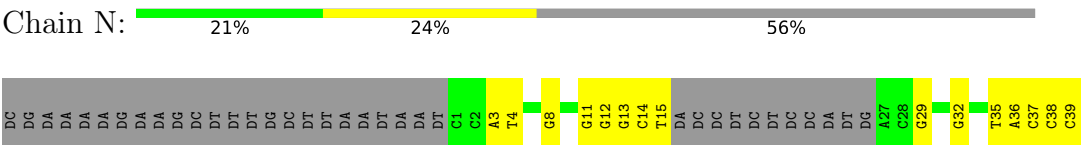
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 53% 32% 14%



TYR	GLY	ALA	E436	L520	R622	1726	A830	I951	L1173	K1271	E1391	L1492	TYR
LEU	LEU	ALA	V437	P521	V623	Q727	G831	D952	L1174	A1272	E1391	L1492	PHE
PHE	ARG	ASP	D438	P522	D624	L728	R832	D953	I1175	V1273	L1395	I1495	ARG
ALA	MET	PRO	L439	R525	V625	F736	E833	A954	S1059	I1274	L1395	I1496	ALA
GLU	PRO	GLU		R525	S626	F736	T834	P957	F1061	S1275	D1399	E1497	GLU
ARG	ARG	GLU	N442	Q529	S629	D739	S835	E958	R1062	E1276	R1406	A1498	GLU
GLU	GLN	GLU	V443	V530	V630	Q744	R836	E959	L1065	I1277	L1407	R1499	GLU
GLY	VAL	VAL	V444	D531	G634	Q744	R838	E959	L1066	E1277	E1410	A1502	VAL
VAL	ARG	ILE	R445	G532	G634	P750	R839	K960	V1067	E1278	P1414	ALA	
ALA	ALA	ALA	V446	G533	G636	Q756	R840	K961	L1068	E1279	V1415	LYS	
GLU	ALA	GLU	S449	R534	Q636	Q756	Y841	Q962	E1069	E1280	A1416	GLY	
LEU	GLN	ALA	V450	F535	G643	Q756	F843	E975	R1078	E1281	P1419	ARG	
LYS	VAL	GLU	D451	D542	L644	I761	N845	L983	D1083	E1282	P1424	ARG	
GLU	ALA	VAL	D452	R545	R646	L764	N845	L983	D1083	E1283	P1424	ARG	
GLU	VAL	VAL	D453	R545	R646	L764	E848	R986	D1083	E1284	P1424	ARG	
GLU	GLU	HIS	A454	R550	L650	H767	E848	R986	D1083	E1285	P1424	ARG	
GLY	GLU	LEU	R455	R550	L650	H767	E848	R986	D1083	E1286	P1424	ARG	
ALA	GLY	ALA	M456	R553	F653	W788	W853	R987	D1083	E1287	P1424	ARG	
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				R553	F653	W788	W853	R987	D1083	E1298	P1424	ARG	
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				R553	F653	W788	W853	R987	D1083	E1300	P1424	ARG	
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				R553	F653	W788	W853	R987	D1083	E1304	P1424	ARG	
				R553	F653	W788	W853	R987	D1083	E1305	P1424	ARG	
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				R553	F653	W788	W853	R987	D1083	E1310	P1424	ARG	
				R553	F653	W788	W853	R987	D1083	E1311	P1424	ARG	
				R553	F653	W788	W853	R987	D1083	E1312	P1424	ARG	
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				R553	F653	W788	W853	R987	D1083	E1392	P1424	ARG	
				R553	F653	W788	W853	R9					

● Molecule 7: nontemplate strand DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24037	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 ($e^-/\text{\AA}^2$)	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	261.4, 261.4, 261.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3069999, 1.3069999, 1.3069999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/1814	0.59	0/2466
1	B	0.40	0/1782	0.58	0/2424
2	C	0.41	0/8937	0.58	0/12087
3	D	0.41	0/10467	0.58	0/14138
4	E	0.41	0/775	0.53	0/1045
5	M	0.38	0/3706	0.63	0/5017
6	T	0.89	0/642	1.24	0/986
7	N	1.05	0/642	1.20	0/986
All	All	0.45	0/28765	0.63	0/39149

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	1782	0	1834	69	0
1	B	1750	0	1797	71	0
2	C	8770	0	8874	307	0
3	D	10293	0	10521	373	0
4	E	761	0	778	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	3635	0	3735	156	0
6	T	574	0	316	33	0
7	N	574	0	316	32	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	28142	0	28171	997	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 18.

The worst 5 of 997 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)
2:C:1086:ARG:HG2	2:C:1111:ILE:CD1	1.50	1.39
1:B:59:GLU:HG3	1:B:139:ASN:HB3	1.19	1.15
2:C:1086:ARG:CG	2:C:1111:ILE:HD12	1.79	1.12
3:D:829:VAL:HG12	3:D:832:ARG:O	1.49	1.11
2:C:1086:ARG:HG2	2:C:1111:ILE:HD12	1.07	1.02

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	224/315 (71%)	214 (96%)	10 (4%)	0	100	100
1	B	220/315 (70%)	202 (92%)	18 (8%)	0	100	100
2	C	1107/1119 (99%)	1041 (94%)	66 (6%)	0	100	100
3	D	1298/1524 (85%)	1221 (94%)	77 (6%)	0	100	100
4	E	92/99 (93%)	87 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	M	453/978 (46%)	399 (88%)	53 (12%)	1 (0%)	47	81
All	All	3394/4350 (78%)	3164 (93%)	229 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	M	663	SER

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	199/273 (73%)	197 (99%)	2 (1%)	76	86
1	B	195/273 (71%)	193 (99%)	2 (1%)	76	86
2	C	936/941 (100%)	928 (99%)	8 (1%)	78	88
3	D	1102/1279 (86%)	1091 (99%)	11 (1%)	76	86
4	E	83/88 (94%)	82 (99%)	1 (1%)	71	84
5	M	383/805 (48%)	380 (99%)	3 (1%)	81	89
All	All	2898/3659 (79%)	2871 (99%)	27 (1%)	79	88

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	419	ASP
3	D	601	ARG
5	M	409	ARG
3	D	486	ARG
3	D	784	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1465	ASN
5	M	684	HIS
4	E	86	GLN
5	M	490	HIS
2	C	829	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](#)

Of 3 ligands modelled in this entry, 3 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

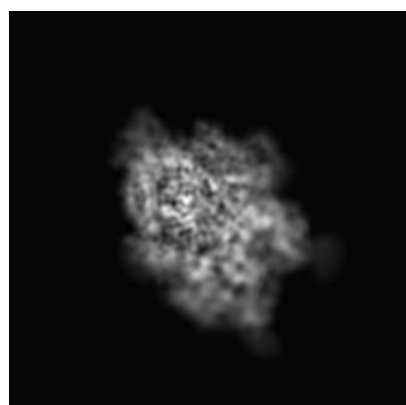
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30117. These allow visual inspection of the internal detail of the map and identification of artifacts.

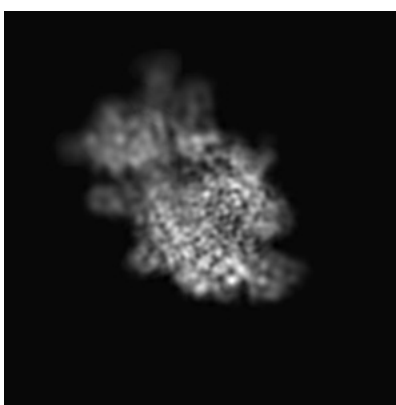
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

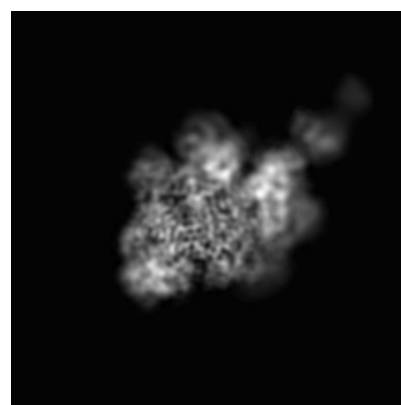
6.1.1 Primary map



X



Y

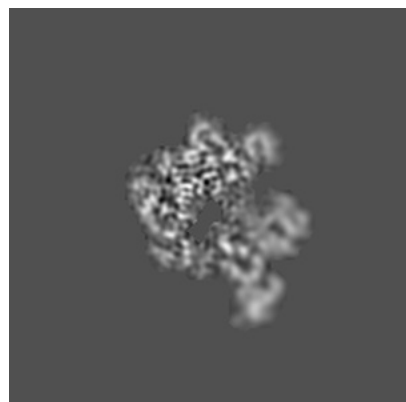


Z

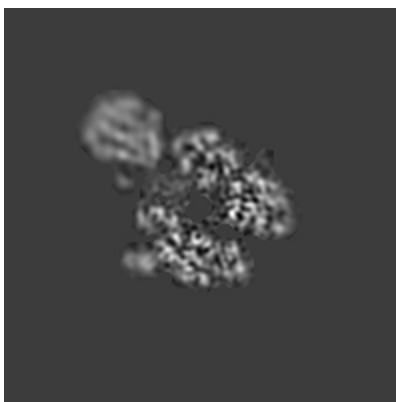
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

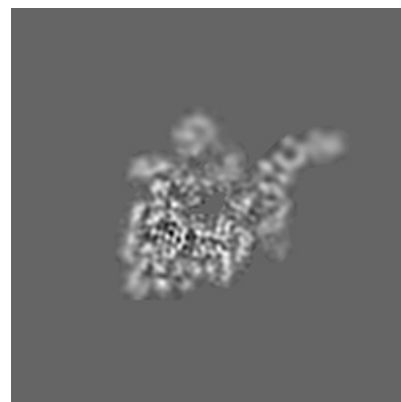
6.2.1 Primary map



X Index: 100



Y Index: 100

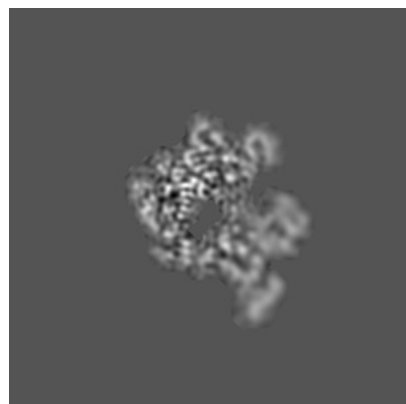


Z Index: 100

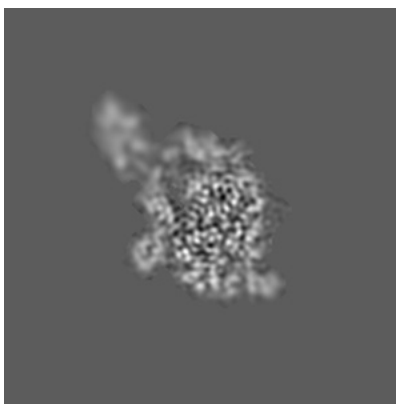
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

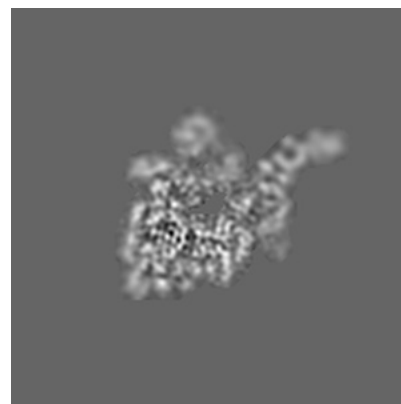
6.3.1 Primary map



X Index: 99



Y Index: 89

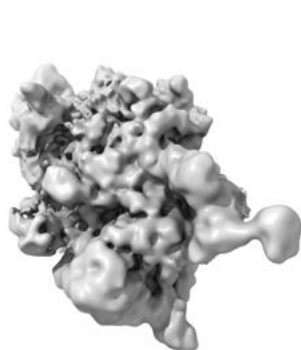


Z Index: 100

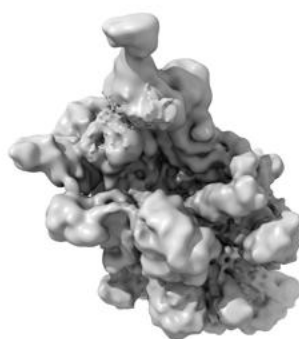
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

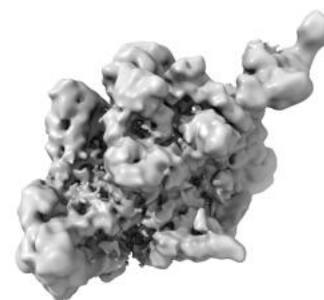
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

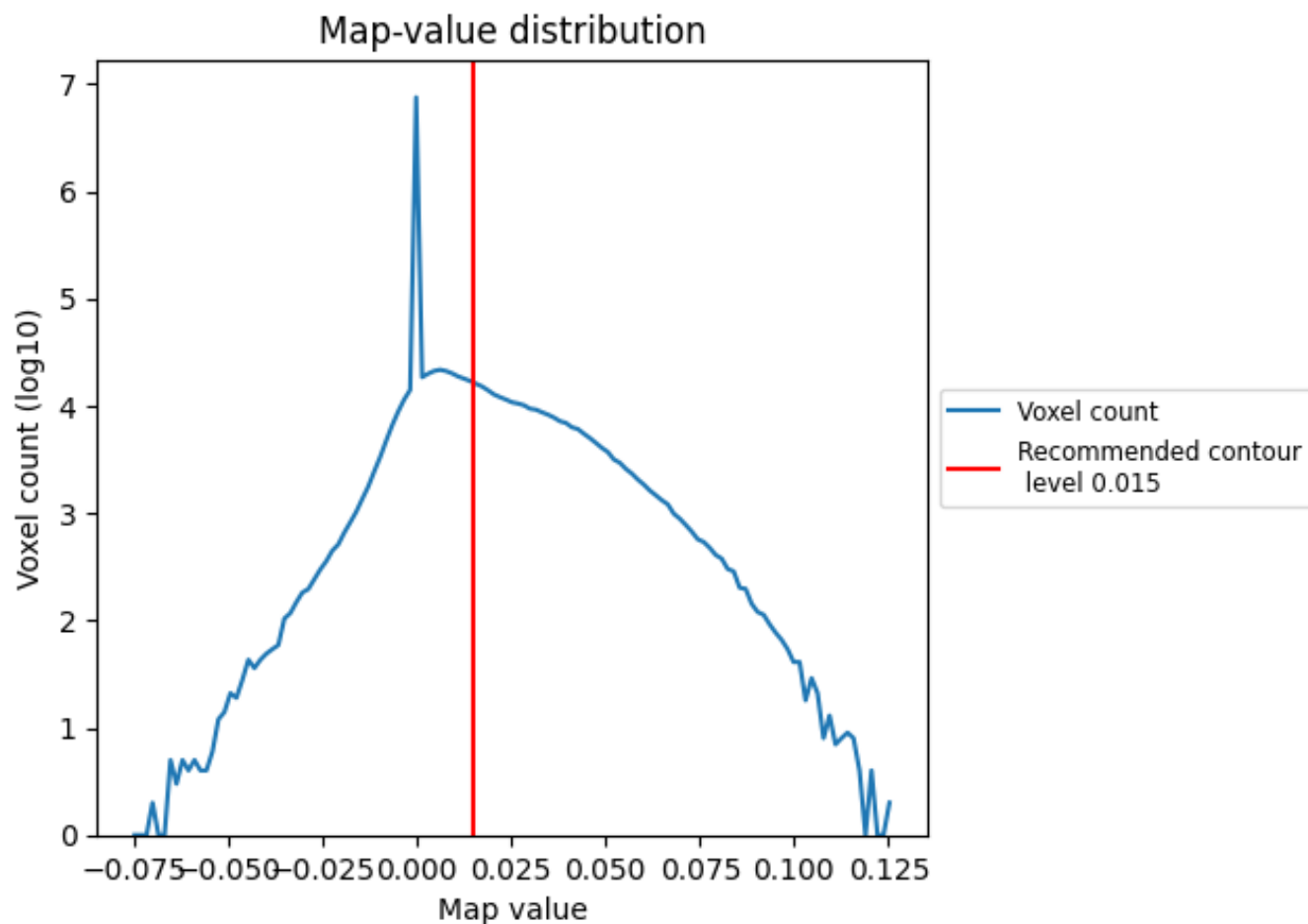
6.5 Mask visualisation

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

7 Map analysis [i](#)

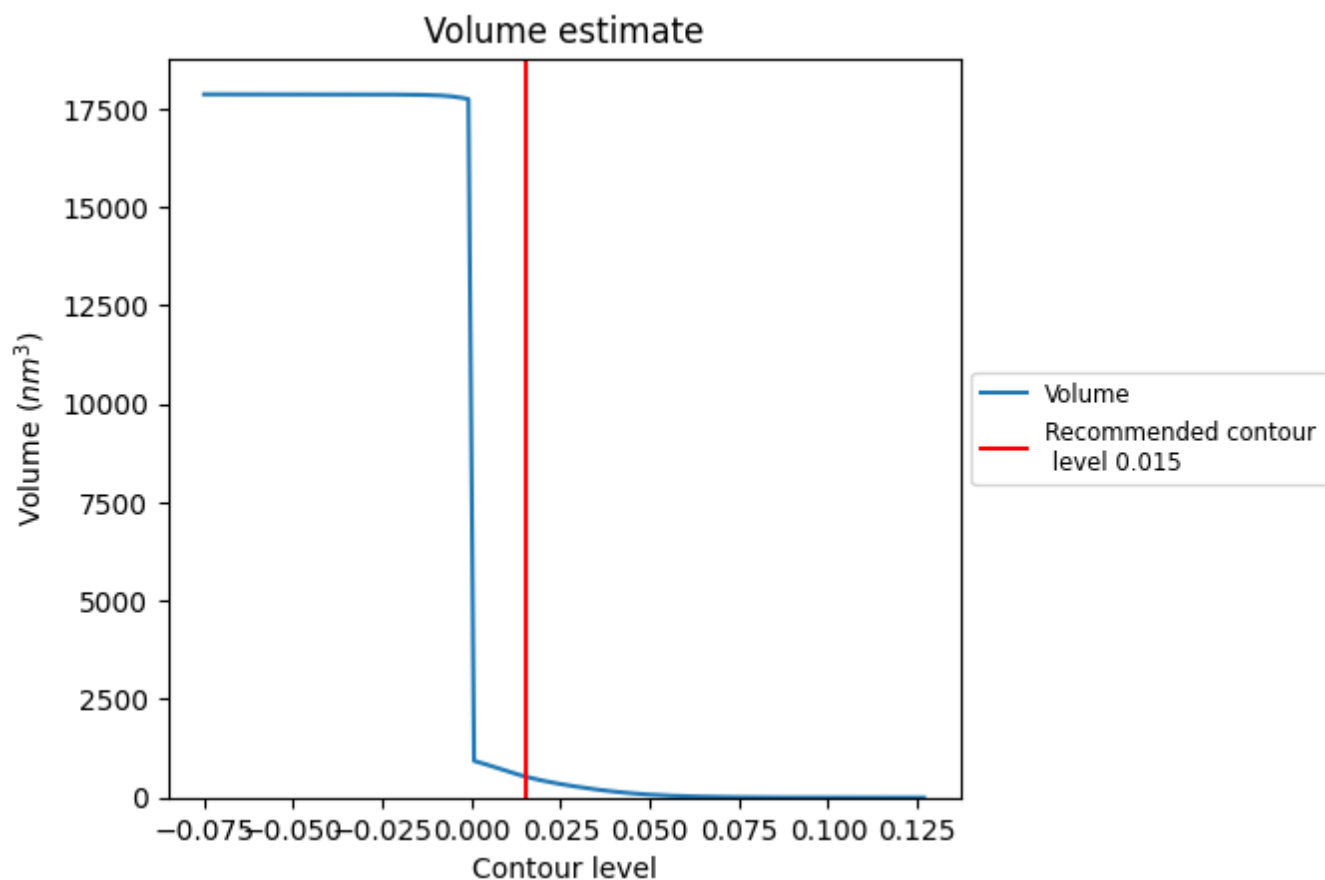
This section contains the results of statistical analysis of the map.

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.

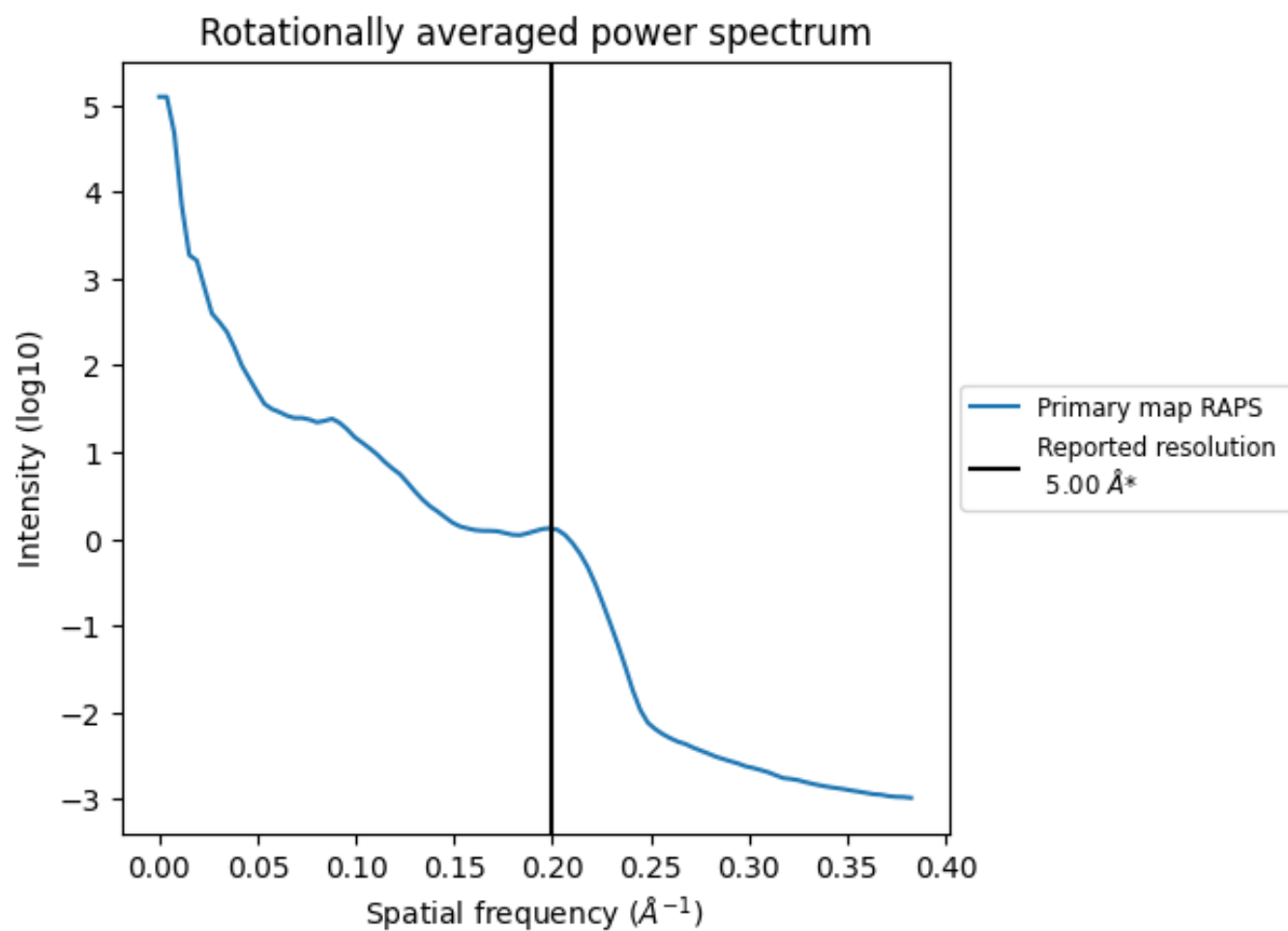
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 537 nm^3 ; this corresponds to an approximate mass of 486 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 0.200 Å⁻¹

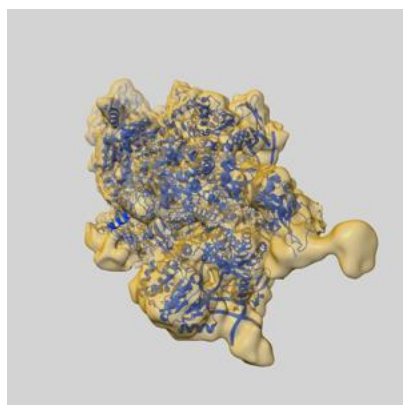
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

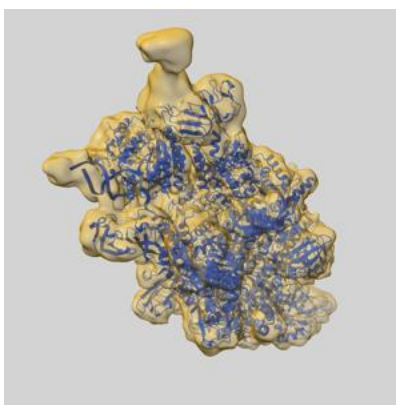
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30117 and PDB model 6M6A. Per-residue inclusion information can be found in section [3](#) on page [5](#).

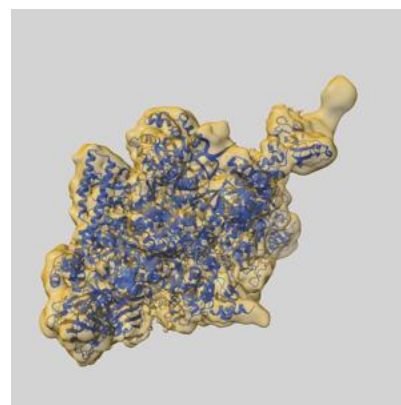
9.1 Map-model overlay [i](#)



X



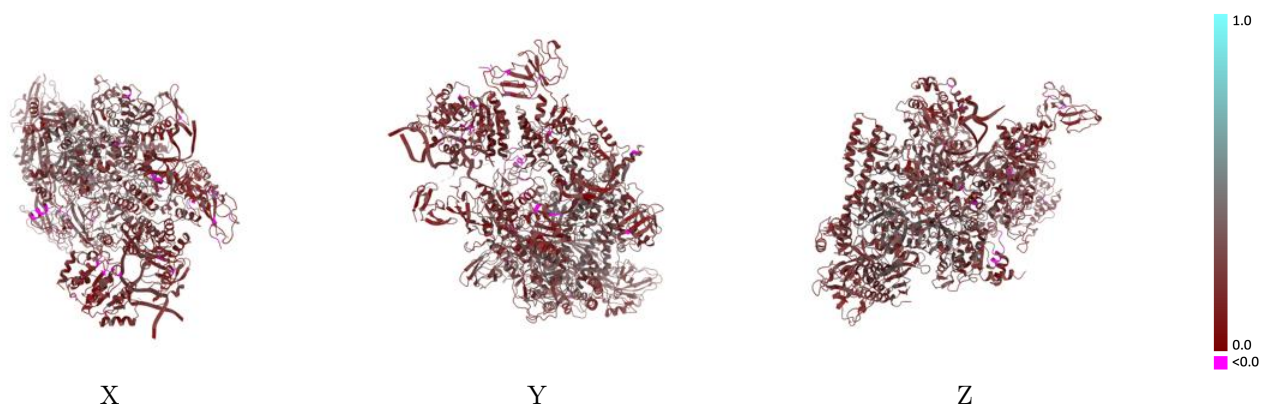
Y



Z

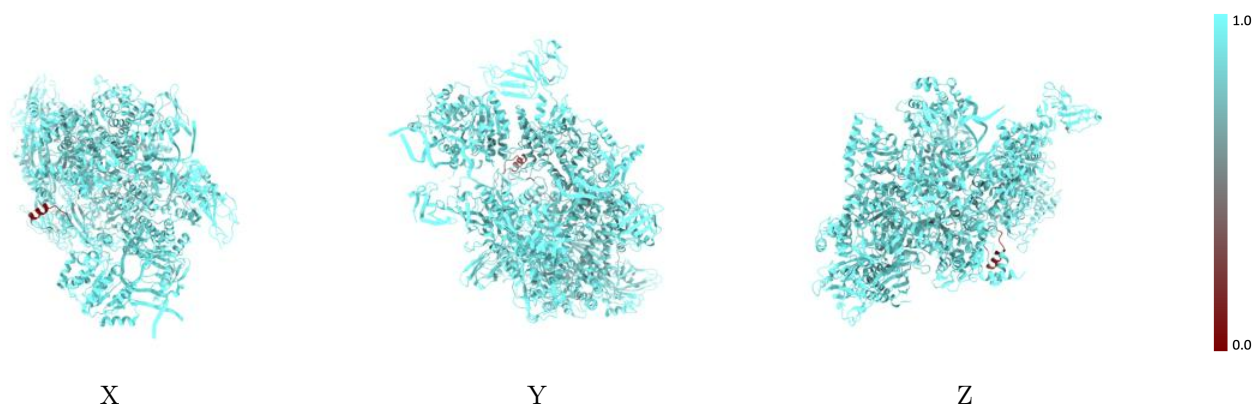
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



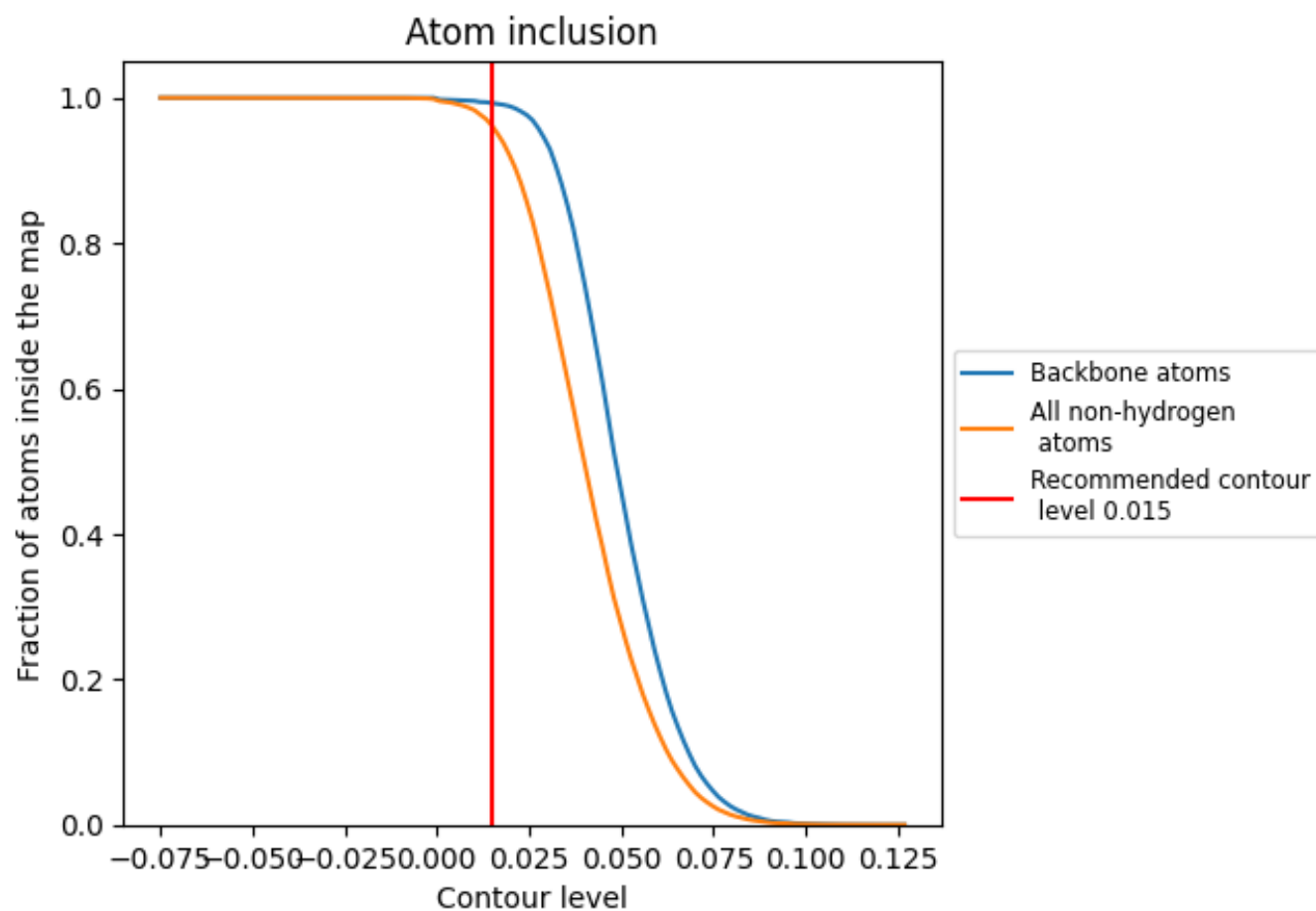
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9615</div>	<div><div></div>0.2560</div>
A	<div><div></div>0.9742</div>	<div><div></div>0.2790</div>
B	<div><div></div>0.9725</div>	<div><div></div>0.2600</div>
C	<div><div></div>0.9470</div>	<div><div></div>0.2700</div>
D	<div><div></div>0.9624</div>	<div><div></div>0.2660</div>
E	<div><div></div>0.9812</div>	<div><div></div>0.2910</div>
M	<div><div></div>0.9697</div>	<div><div></div>0.1860</div>
N	<div><div></div>0.9895</div>	<div><div></div>0.2090</div>
T	<div><div></div>0.9843</div>	<div><div></div>0.2100</div>

1.0

0.0

<0.0