



wwPDB EM Validation Summary Report ⓘ

Feb 24, 2025 – 12:23 PM EST

PDB ID : 9EI1
EMDB ID : EMD-48073
Title : Cryo-EM structure of Human RNA polymerase II Elongation Complex bound to the RECQL5 helicase in the absence of nucleotide
Authors : Florez Ariza, A.; Lue, N.; Nogales, E.
Deposited on : 2024-11-25
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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

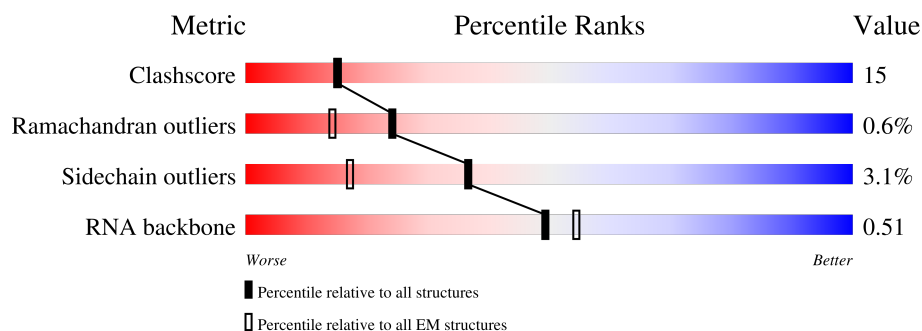
1 Overall quality at a glance

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.





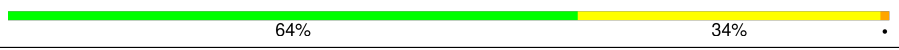

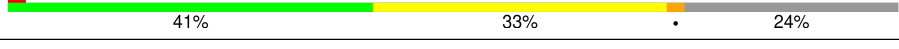


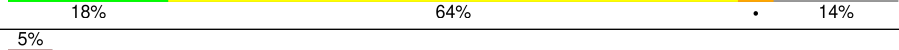
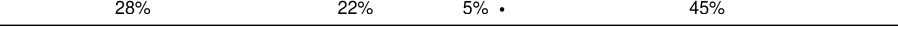
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1970	
2	B	1174	
3	C	275	
4	D	142	
5	E	210	
6	F	127	
7	G	172	

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Mol	Chain	Length	Quality of chain
8	H	150	
9	I	125	
10	J	67	
11	K	117	
12	L	58	
13	N	43	
14	P	20	
15	T	28	
16	U	991	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 36623 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1442	Total	C	N	O	S	0	0
			11431	7188	2044	2126	73		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1134	Total	C	N	O	S	0	0
			9062	5732	1595	1671	64		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	257	Total	C	N	O	S	0	0
			2060	1296	351	407	6		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	128	Total	C	N	O	S	0	0
			1005	632	172	197	4		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	209	Total	C	N	O	S	0	0
			1711	1084	300	319	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	PHE	SER	conflict	UNP P19388

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			658	419	113	121	5		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1334	867	216	243	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	0
			920	593	152	173	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 13 is a DNA chain called Non-template DNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	22	Total	C	N	O	P	0	0
			455	217	86	130	22		

- Molecule 14 is a RNA chain called RNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	11	Total	C	N	O	P	0	0
			239	107	49	72	11		

- Molecule 15 is a DNA chain called Template DNA, nucleic acid scaffold.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	24	Total	C	N	O	P	0	0
			486	233	82	147	24		

- Molecule 16 is a protein called ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	545	Total	C	N	O	S	0	0
			4235	2673	756	779	27		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	157	ALA	ASP	engineered mutation	UNP O94762

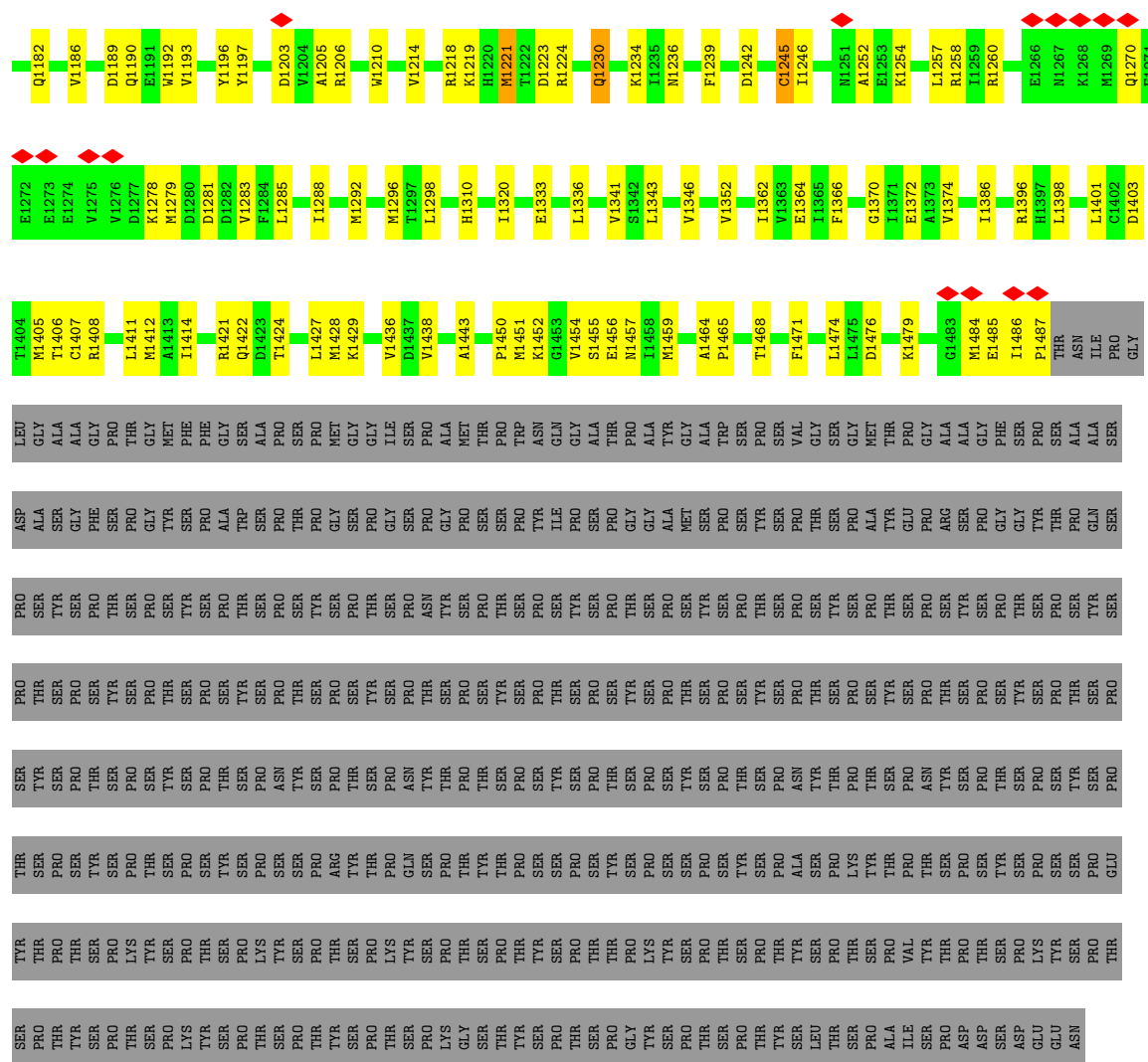
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	A	2	Total	Zn	0
			2	2	
17	B	1	Total	Zn	0
			1	1	
17	C	1	Total	Zn	0
			1	1	
17	I	2	Total	Zn	0
			2	2	
17	J	1	Total	Zn	0
			1	1	
17	L	1	Total	Zn	0
			1	1	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Lig-

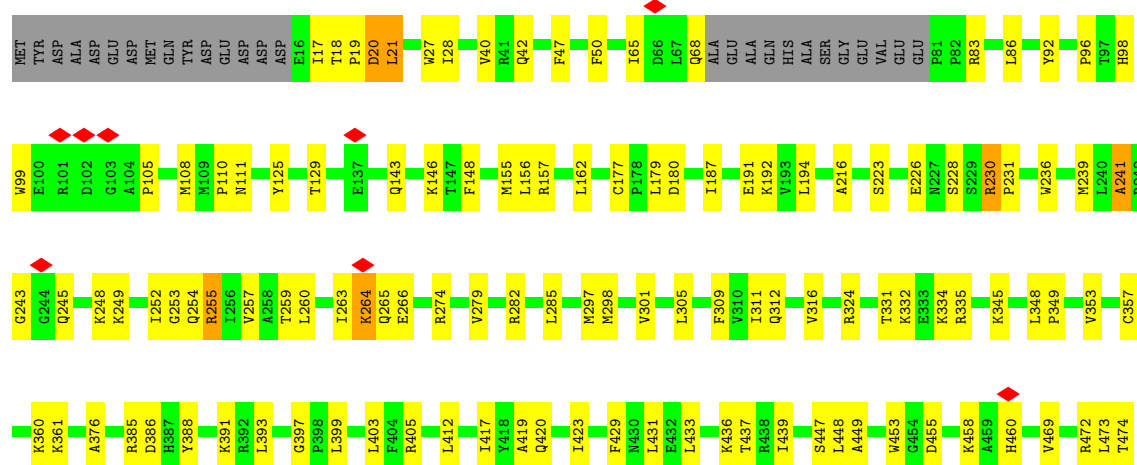
and of Interest" by depositor).

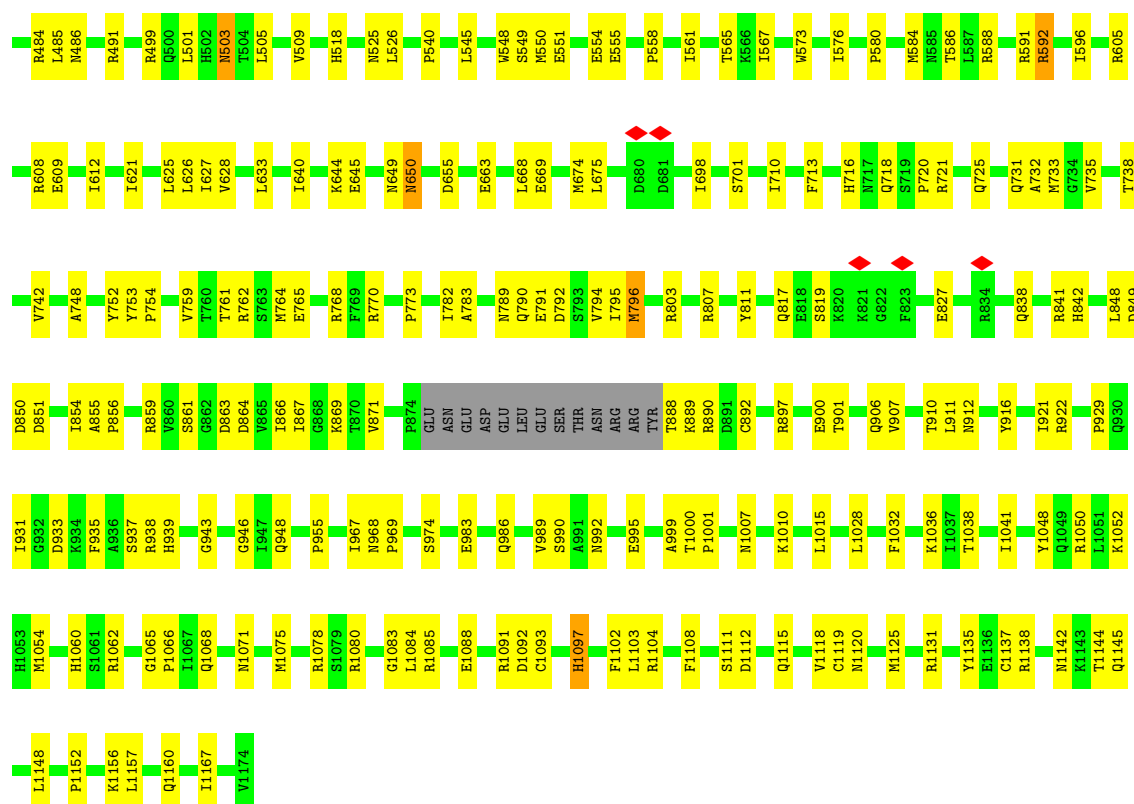
Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	



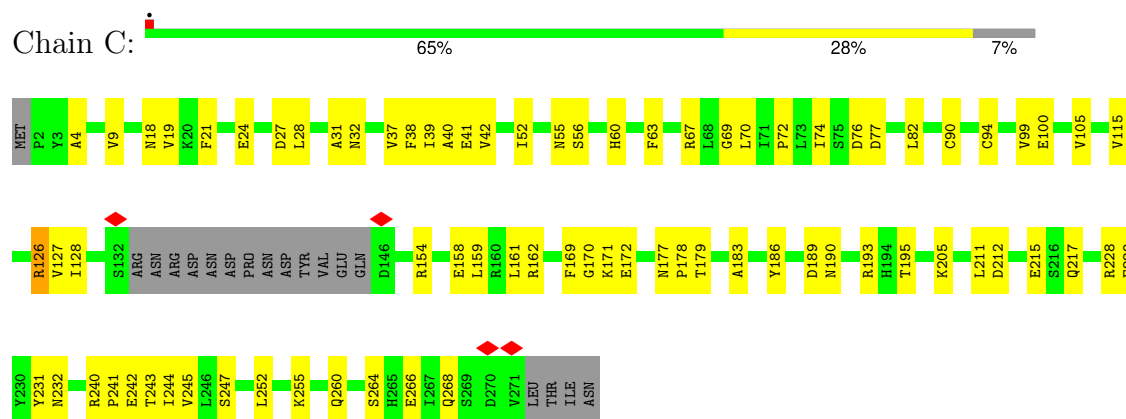
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B: 69% 27%






• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

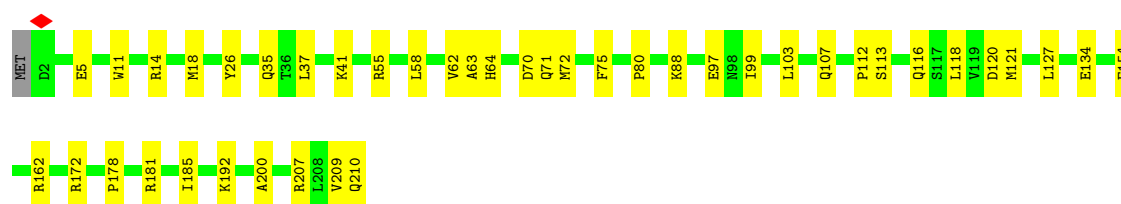


• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



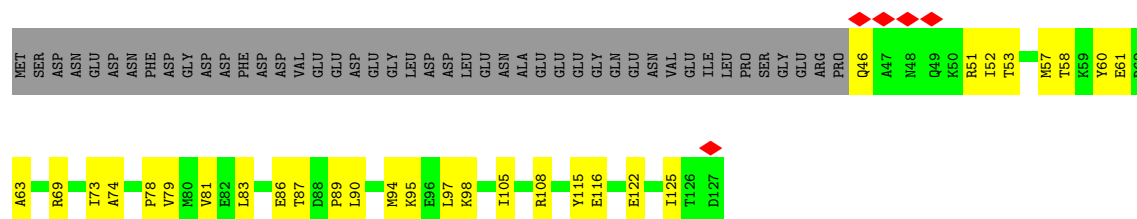
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:  80% 20%



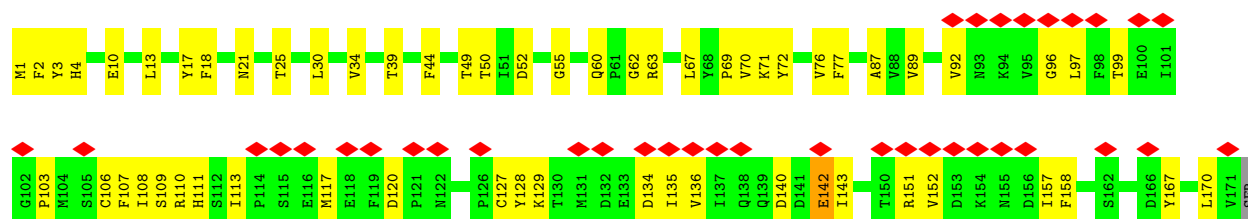
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  41% 24% 35%



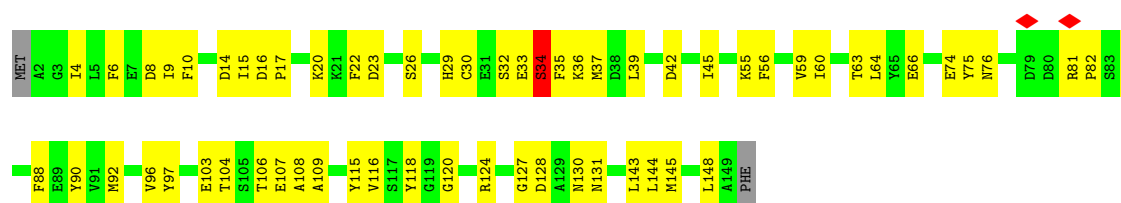
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:  22% 65% 34%



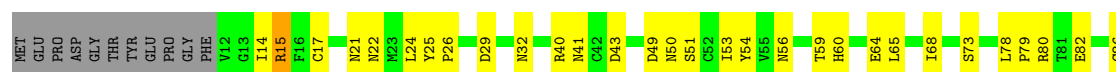
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  58% 40%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:  56% 33% 9%





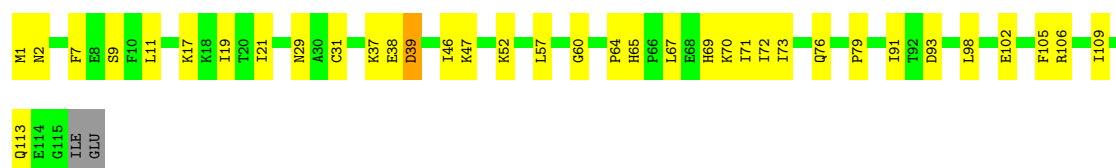
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 64% 34%



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a

Chain K: 68% 30%



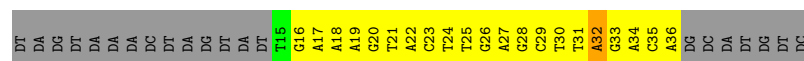
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 41% 33% 24%



- Molecule 13: Non-template DNA, nucleic acid scaffold

Chain N: 47% 49%



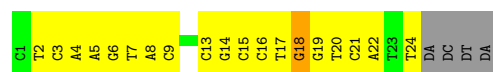
- Molecule 14: RNA, nucleic acid scaffold

Chain P: 15% 25% 10% 5% 45%



- Molecule 15: Template DNA, nucleic acid scaffold

Chain T: 18% 64% 14%



- Molecule 16: ATP-dependent DNA helicase Q5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24323	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.830	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: 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	0.27	0/11641	0.52	1/15715 (0.0%)
2	B	0.28	0/9243	0.52	1/12475 (0.0%)
3	C	0.28	0/2103	0.48	0/2858
4	D	0.24	0/1019	0.57	1/1374 (0.1%)
5	E	0.29	0/1742	0.55	1/2353 (0.0%)
6	F	0.29	0/668	0.58	0/903
7	G	0.29	0/1365	0.55	1/1853 (0.1%)
8	H	0.29	0/1207	0.53	0/1628
9	I	0.30	0/948	0.54	0/1284
10	J	0.28	0/542	0.51	0/730
11	K	0.28	0/939	0.48	0/1271
12	L	0.34	0/377	0.76	1/500 (0.2%)
13	N	0.65	0/511	1.19	3/787 (0.4%)
14	P	0.49	0/268	1.26	5/416 (1.2%)
15	T	0.55	0/542	0.98	1/833 (0.1%)
16	U	0.36	0/4313	0.62	1/5826 (0.0%)
All	All	0.31	0/37428	0.57	16/50806 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
16	U	0	8

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	11	A	C3'-C2'-C1'	-8.43	94.76	101.50
12	L	33	PRO	CA-N-CD	-8.32	99.85	111.50
1	A	526	VAL	C-N-CA	8.22	142.26	121.70
4	D	88	LEU	CA-CB-CG	7.52	132.59	115.30
5	E	80	PRO	CA-N-CD	-7.43	101.09	111.50

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	U	109	ARG	Sidechain
16	U	118	ARG	Sidechain
16	U	131	GLU	Mainchain
16	U	180	ARG	Sidechain
16	U	182	ARG	Sidechain

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	11431	0	11539	322	0
2	B	9062	0	9107	222	0
3	C	2060	0	2011	58	0
4	D	1005	0	964	40	0
5	E	1711	0	1729	31	0
6	F	658	0	686	25	0
7	G	1334	0	1333	35	0
8	H	1186	0	1147	47	0
9	I	927	0	859	31	0
10	J	533	0	553	21	0
11	K	920	0	942	25	0
12	L	372	0	378	20	0
13	N	455	0	248	63	0
14	P	239	0	121	20	0
15	T	486	0	273	23	0
16	U	4235	0	4233	265	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	36623	0	36123	1066	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 15.

The worst 5 of 1066 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)
13:N:34:DA:C1'	16:U:131:GLU:HB3	1.15	1.57
13:N:34:DA:C1'	16:U:131:GLU:CB	2.00	1.38
13:N:36:DA:C5'	16:U:103:LYS:HZ3	1.38	1.37
13:N:27:DA:N1	15:T:2:DT:N3	1.70	1.33
13:N:34:DA:H1'	16:U:131:GLU:CB	1.58	1.31

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	1434/1970 (73%)	1364 (95%)	69 (5%)	1 (0%)	48	80
2	B	1128/1174 (96%)	1068 (95%)	58 (5%)	2 (0%)	44	75
3	C	253/275 (92%)	242 (96%)	11 (4%)	0	100	100
4	D	126/142 (89%)	123 (98%)	3 (2%)	0	100	100
5	E	207/210 (99%)	194 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	80/127 (63%)	79 (99%)	1 (1%)	0	100	100
7	G	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
8	H	146/150 (97%)	138 (94%)	7 (5%)	1 (1%)	19	54
9	I	112/125 (90%)	101 (90%)	10 (9%)	1 (1%)	14	49
10	J	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
11	K	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
12	L	42/58 (72%)	38 (90%)	4 (10%)	0	100	100
16	U	535/991 (54%)	438 (82%)	77 (14%)	20 (4%)	2	19
All	All	4410/5578 (79%)	4117 (93%)	268 (6%)	25 (1%)	24	57

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	U	83	ILE
16	U	84	GLN
16	U	101	ASN
16	U	130	PRO
16	U	157	ALA

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	1270/1748 (73%)	1247 (98%)	23 (2%)	54	77
2	B	993/1028 (97%)	977 (98%)	16 (2%)	58	79
3	C	234/252 (93%)	232 (99%)	2 (1%)	75	89
4	D	106/126 (84%)	105 (99%)	1 (1%)	75	89
5	E	189/192 (98%)	188 (100%)	1 (0%)	86	93
6	F	71/111 (64%)	68 (96%)	3 (4%)	25	58
7	G	147/153 (96%)	142 (97%)	5 (3%)	32	63
8	H	129/131 (98%)	127 (98%)	2 (2%)	58	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	103/112 (92%)	97 (94%)	6 (6%)	17	49
10	J	56/56 (100%)	52 (93%)	4 (7%)	12	42
11	K	104/106 (98%)	101 (97%)	3 (3%)	37	67
12	L	41/55 (74%)	40 (98%)	1 (2%)	44	71
16	U	448/819 (55%)	393 (88%)	55 (12%)	4	19
All	All	3891/4889 (80%)	3769 (97%)	122 (3%)	37	66

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	118	HIS
16	U	319	PHE
16	U	103	LYS
16	U	304	ASP
16	U	385	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
16	U	185	HIS
16	U	107	GLN
2	B	1068	GLN
9	I	100	HIS
2	B	1021	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	10/20 (50%)	3 (30%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	11	A
14	P	12	A
14	P	13	G

There are no RNA pucker outliers to report.

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](#)

Of 9 ligands modelled in this entry, 9 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.

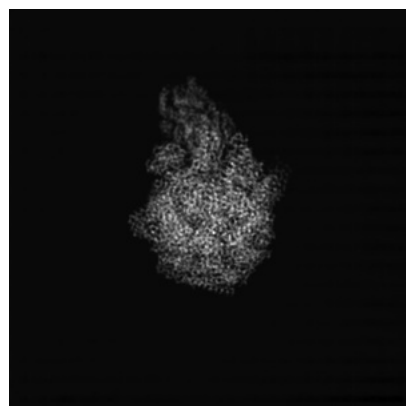
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48073. These allow visual inspection of the internal detail of the map and identification of artifacts.

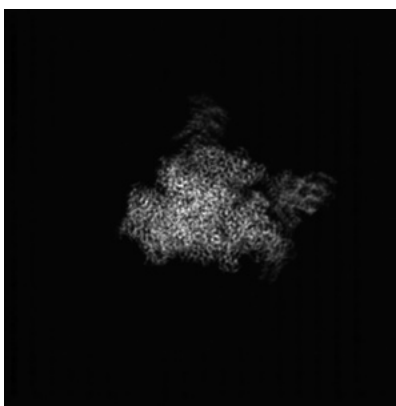
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

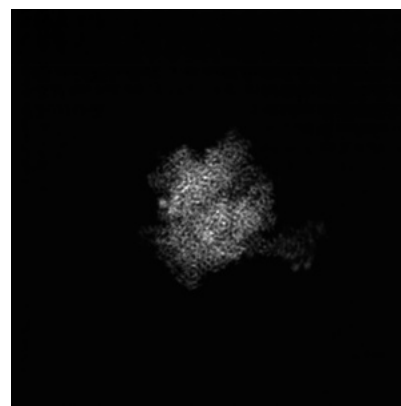
6.1.1 Primary map



X

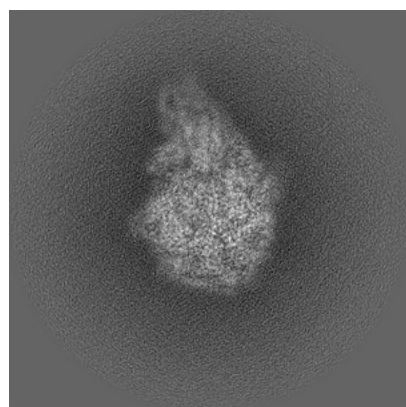


Y

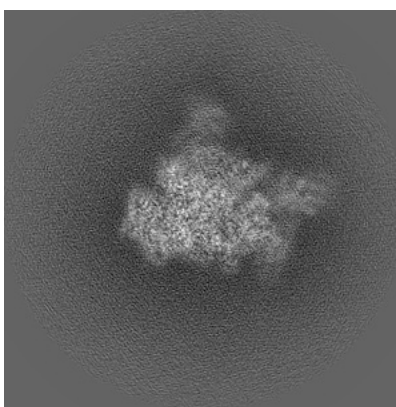


Z

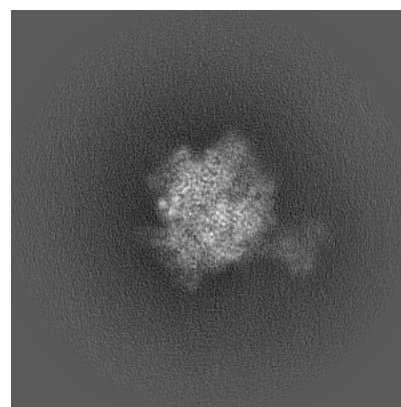
6.1.2 Raw map



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: 160

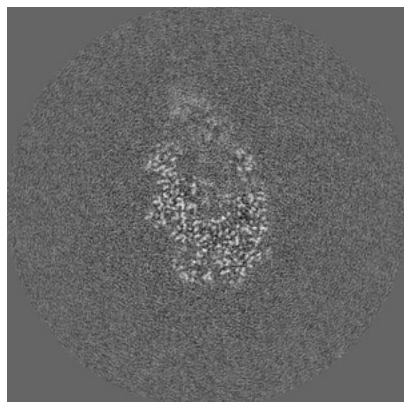


Y Index: 160

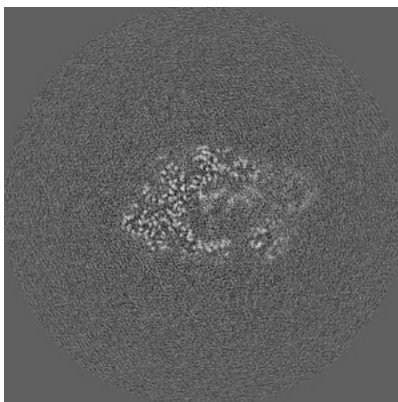


Z Index: 160

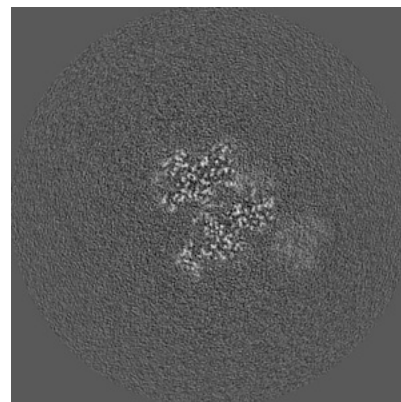
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 159

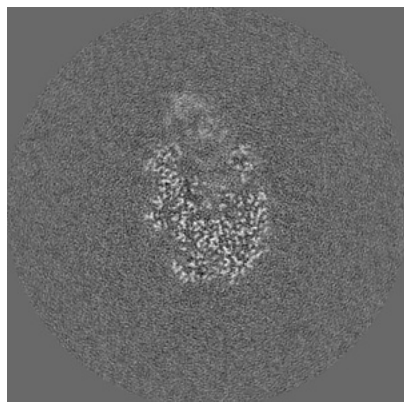


Y Index: 157

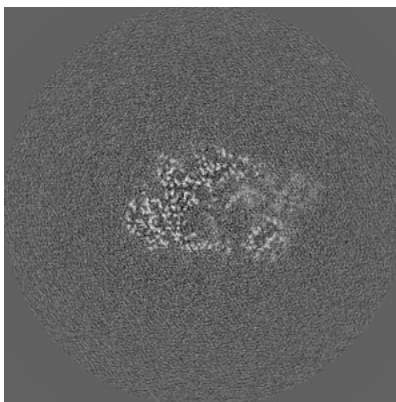


Z Index: 161

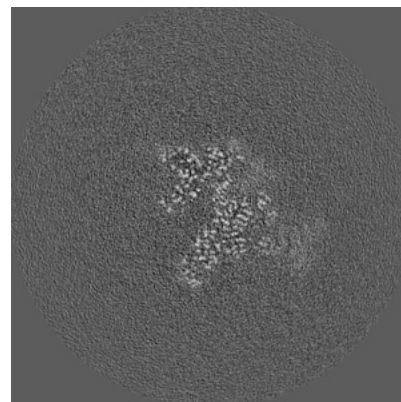
6.3.2 Raw map



X Index: 159



Y Index: 158

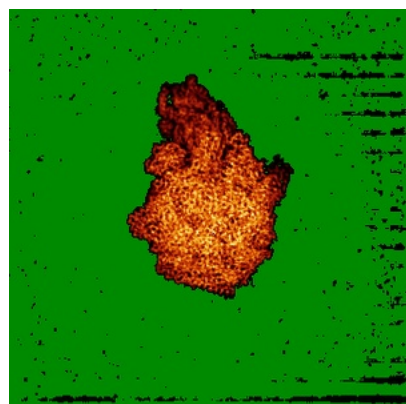


Z Index: 153

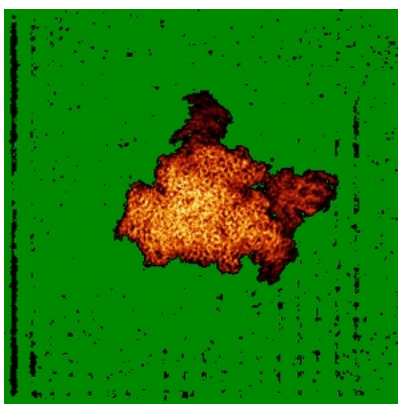
The images above show the largest variance slices of the map in three orthogonal directions.

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

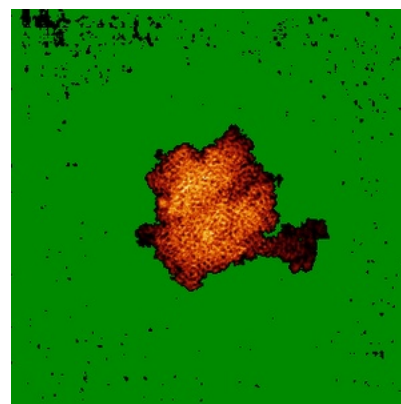
6.4.1 Primary map



X

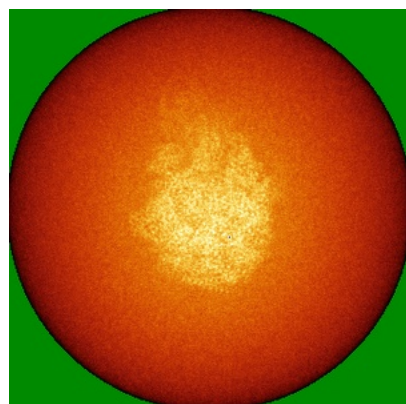


Y

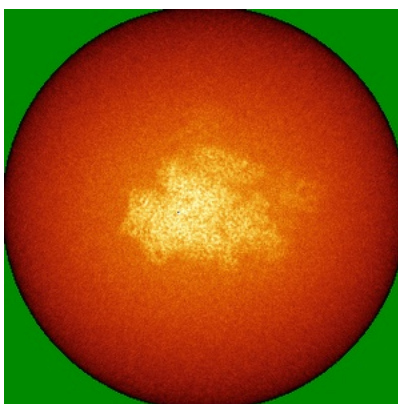


Z

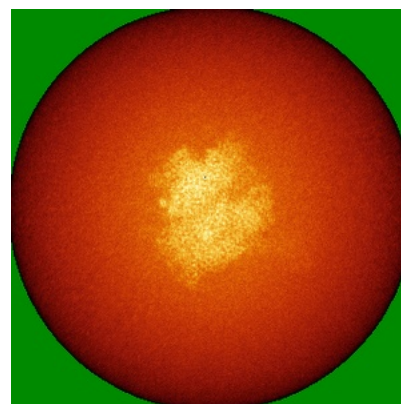
6.4.2 Raw map



X



Y

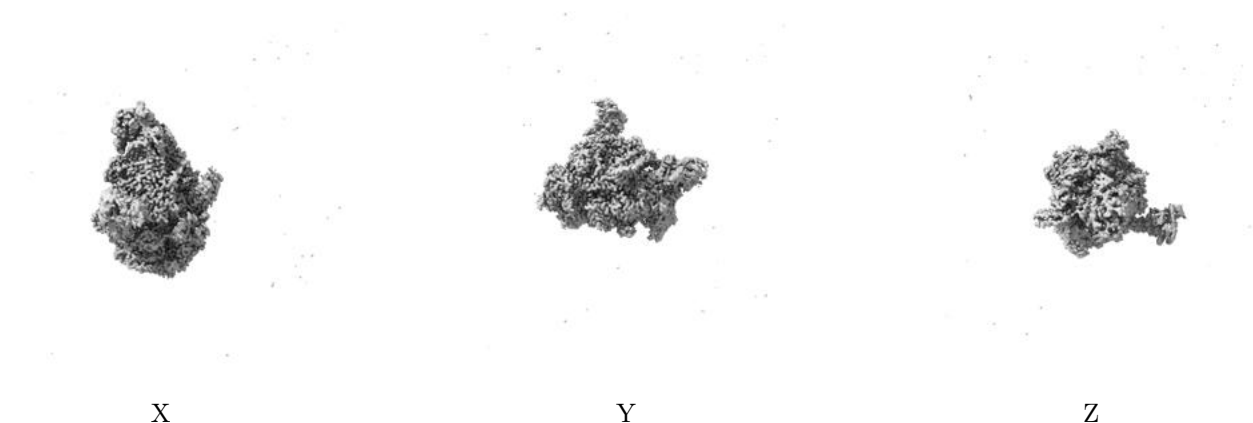


Z

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.

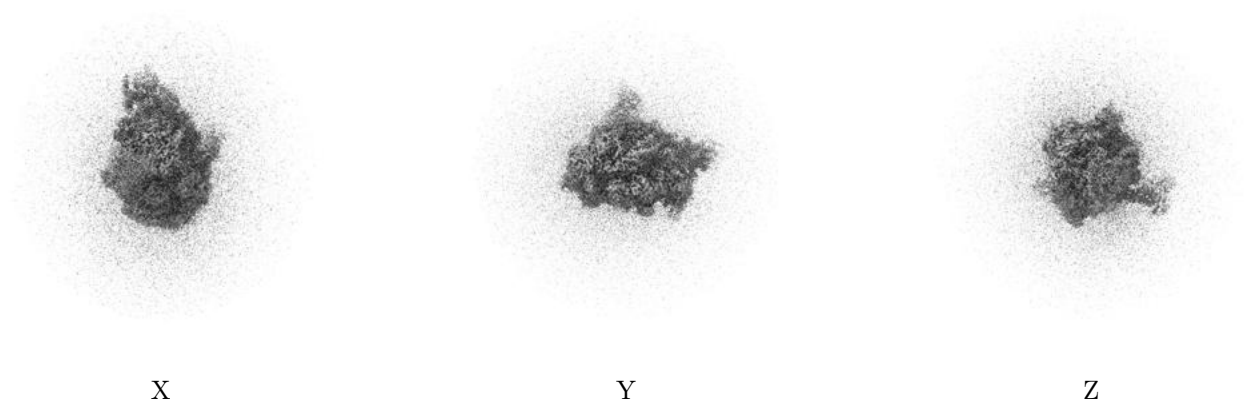
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

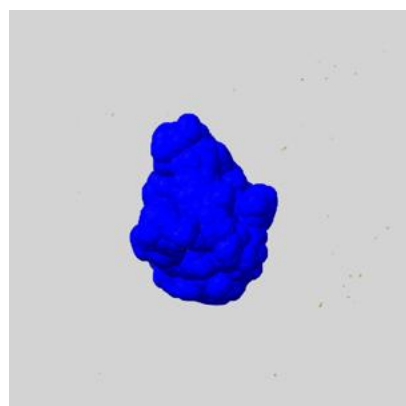
6.6 Mask visualisation [i](#)

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

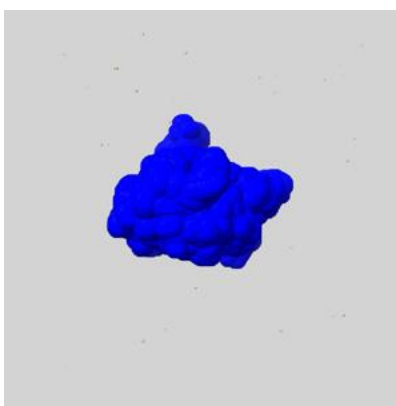
A mask typically either:

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

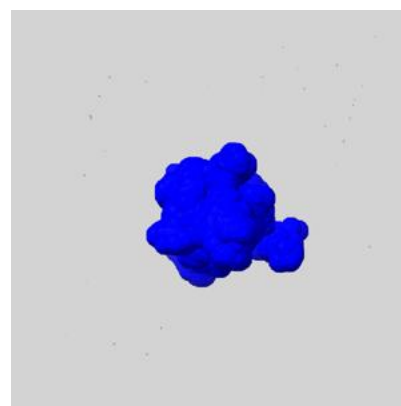
6.6.1 emd_48073_msk_1.map [i](#)



X



Y

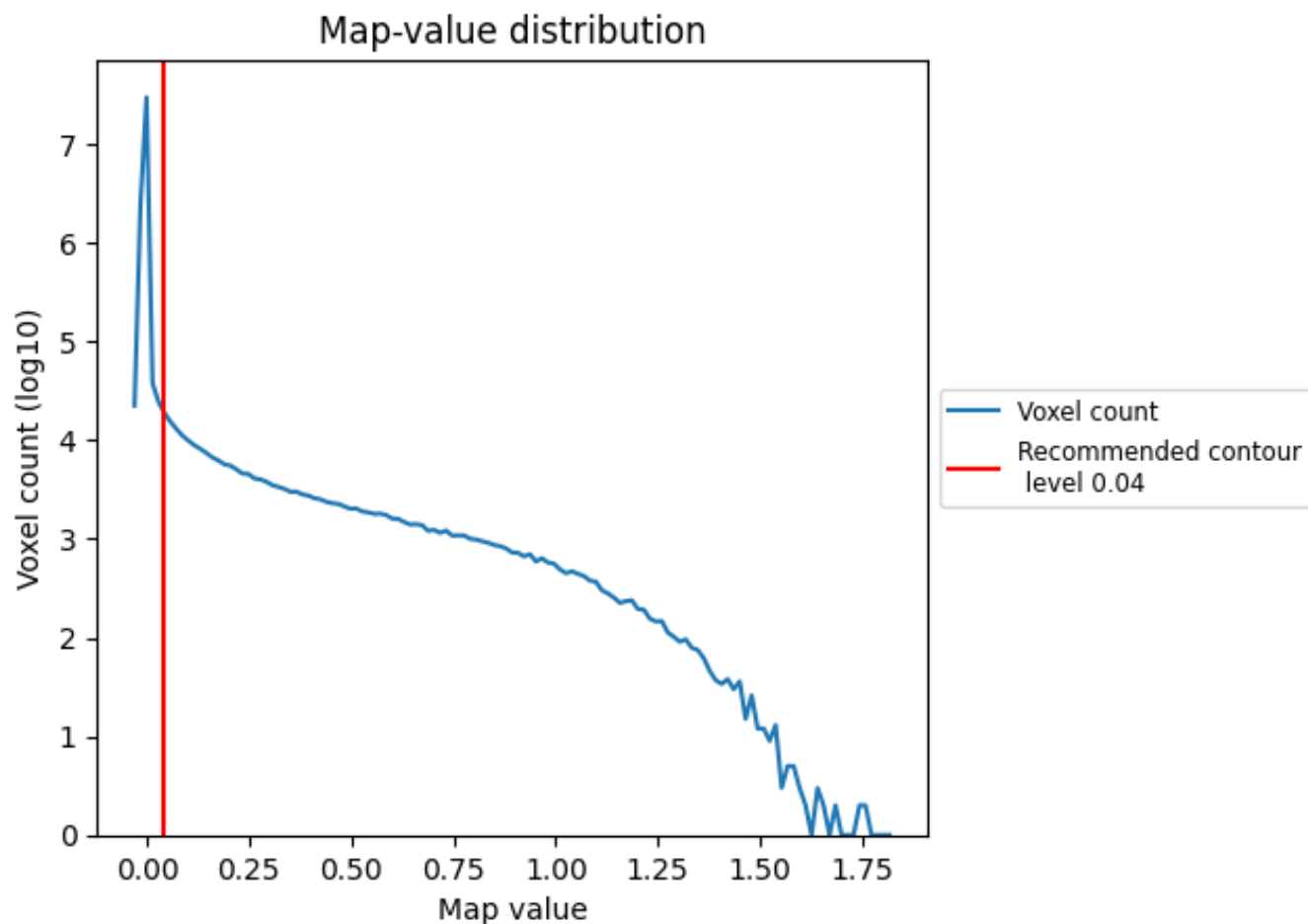


Z

7 Map analysis [i](#)

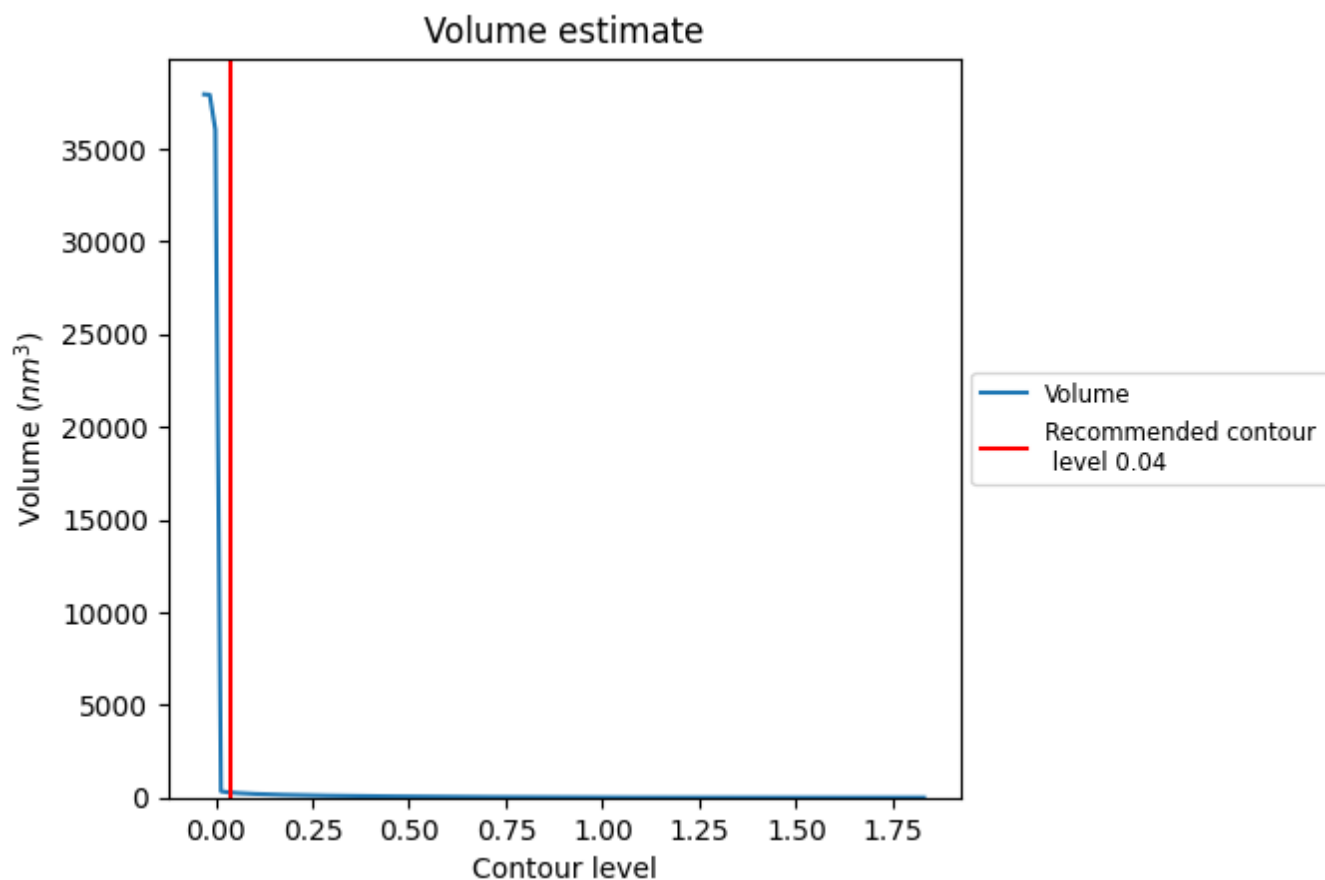
This section contains the results of statistical analysis of the map.

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.

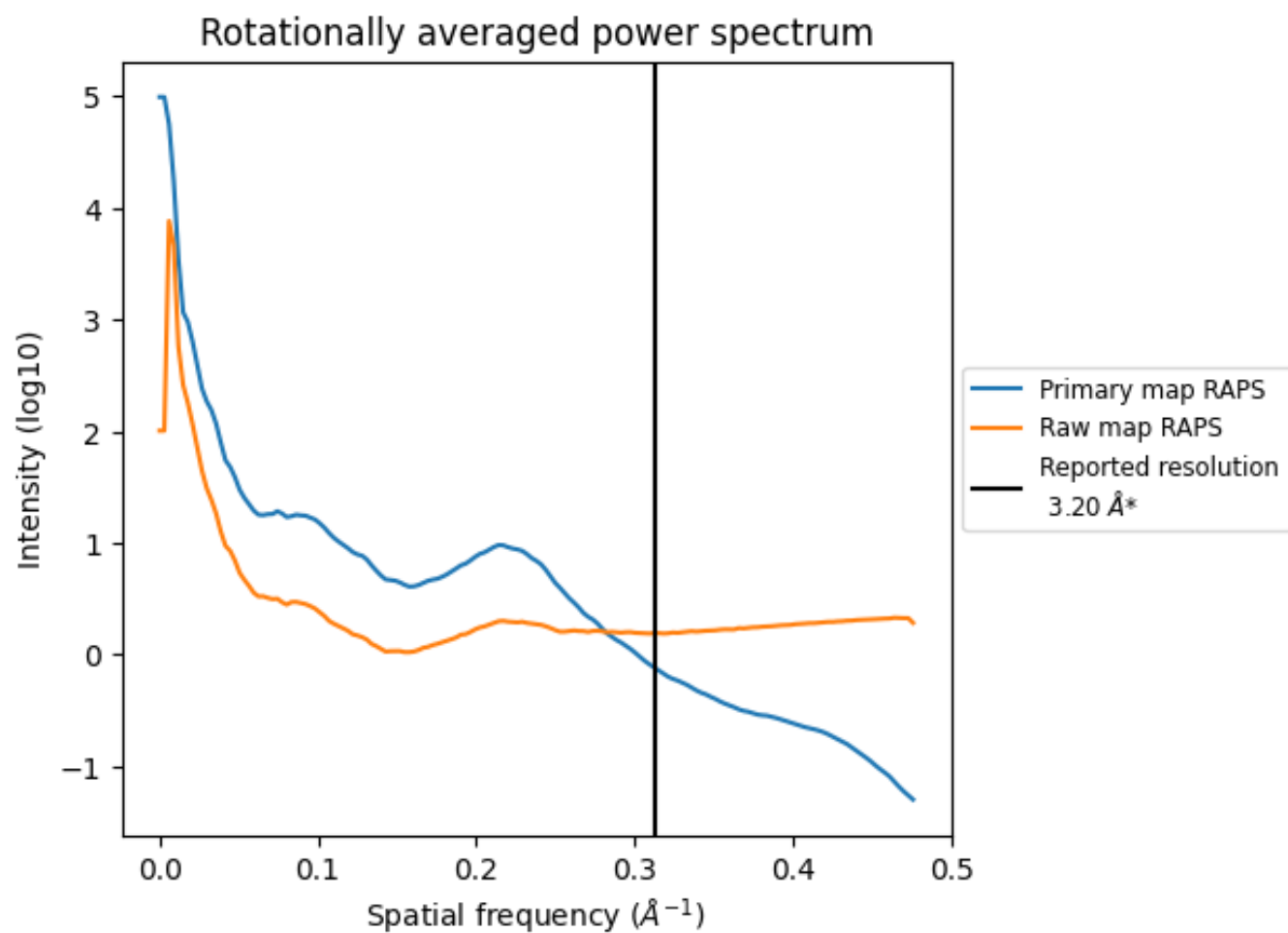
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 270 nm^3 ; this corresponds to an approximate mass of 244 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 ⓘ

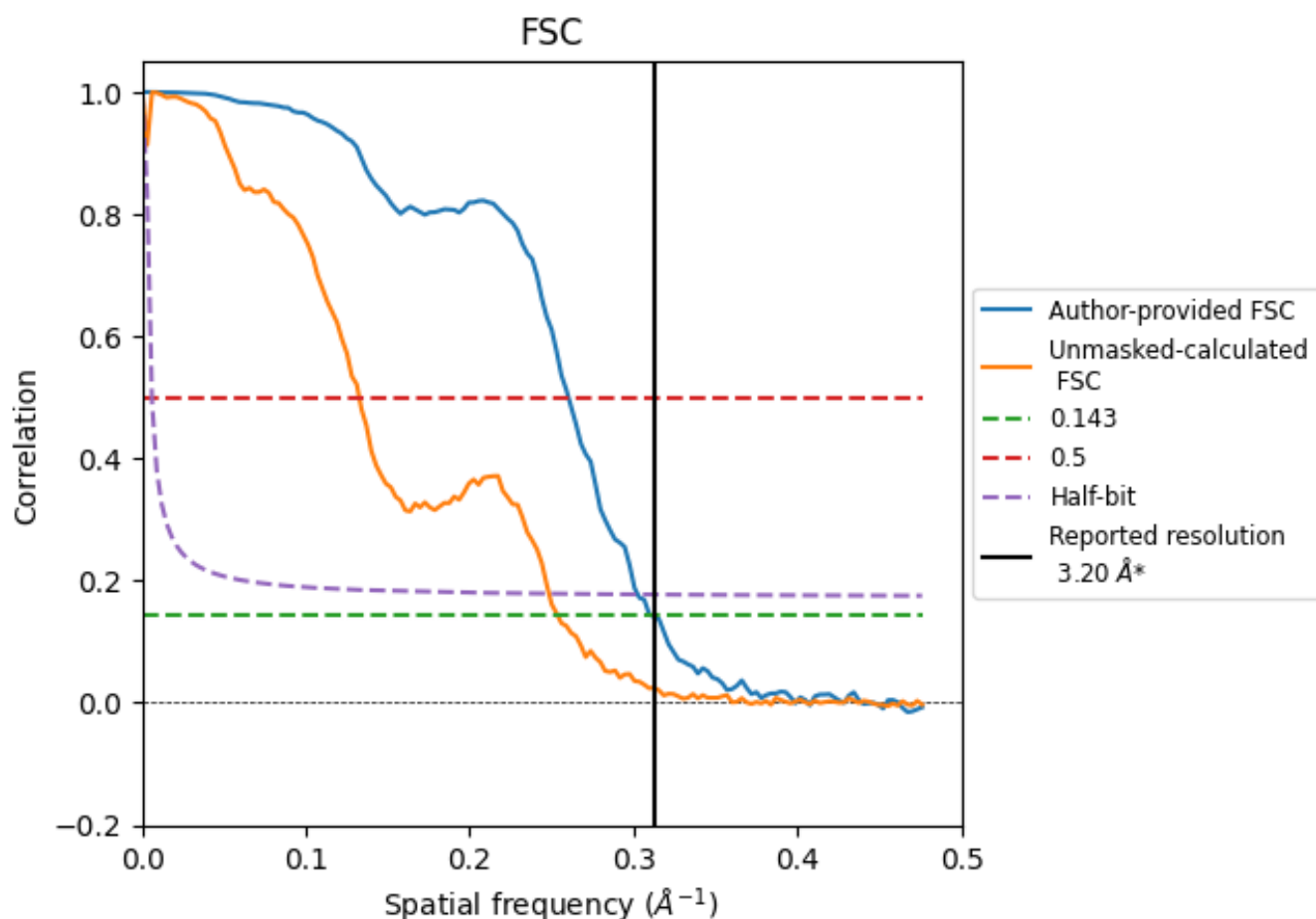


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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](#)

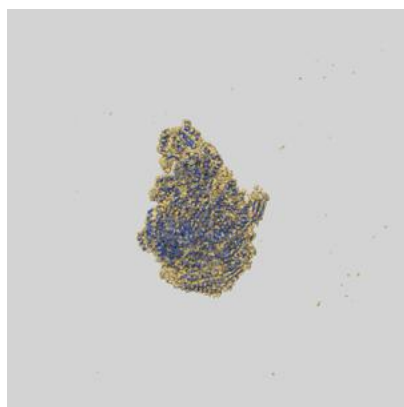
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.84	3.31
Unmasked-calculated*	3.94	7.55	4.03

*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 3.94 differs from the reported value 3.2 by more than 10 %

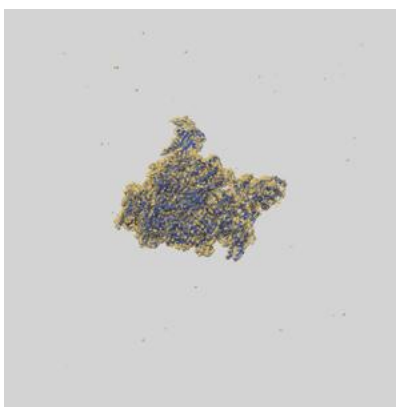
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-48073 and PDB model 9EI1. Per-residue inclusion information can be found in section [3](#) on page [8](#).

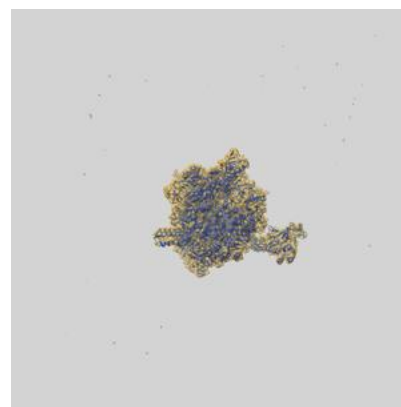
9.1 Map-model overlay [i](#)



X



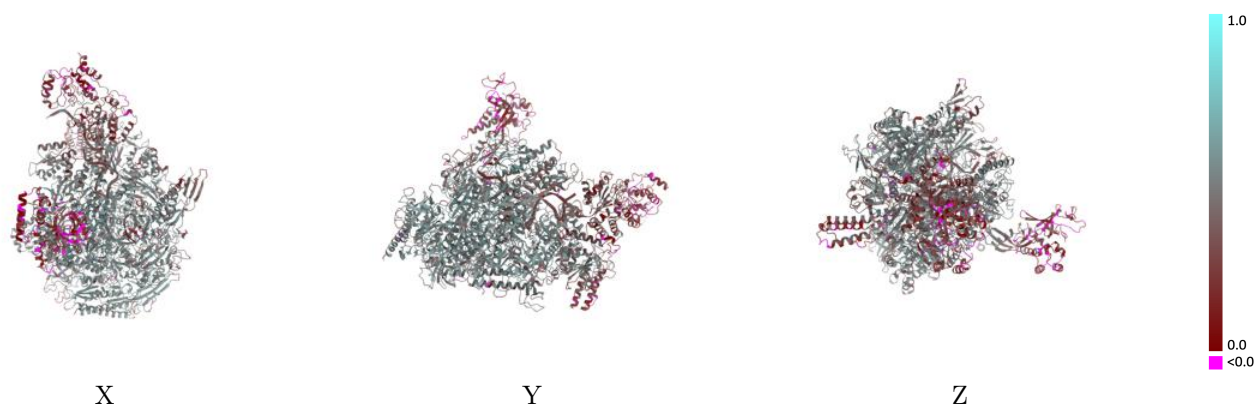
Y



Z

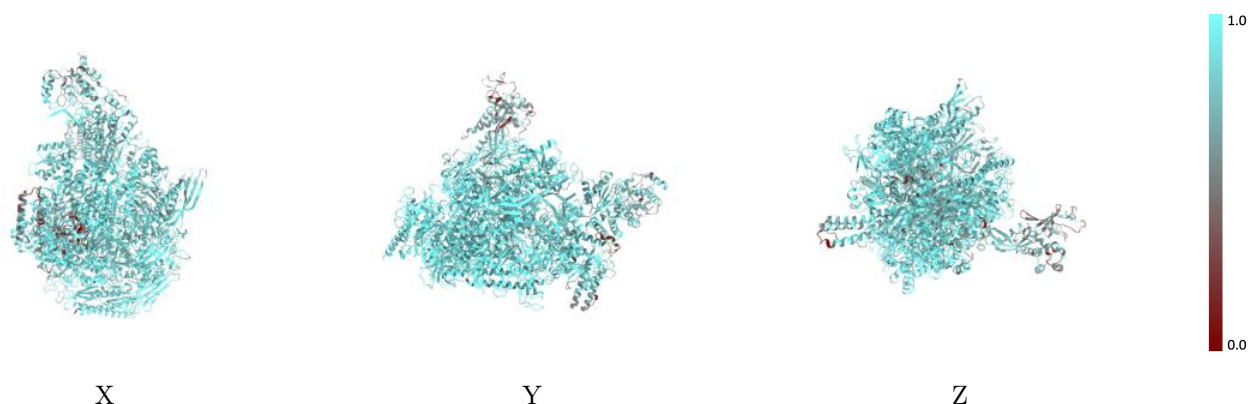
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



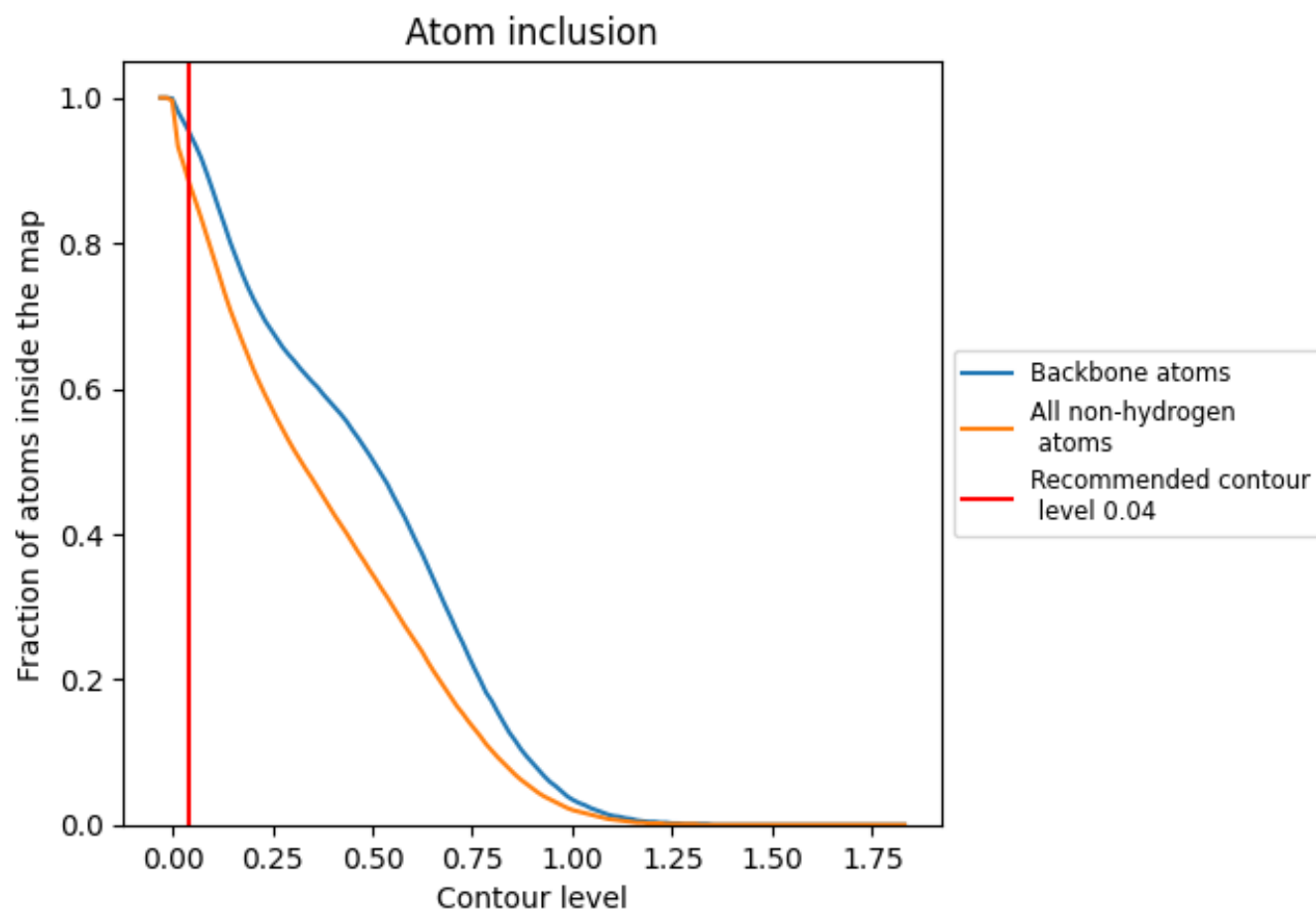
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8860	 0.4420
A	 0.9280	 0.4940
B	 0.9340	 0.4990
C	 0.9350	 0.5140
D	 0.5940	 0.1350
E	 0.9230	 0.4740
F	 0.9030	 0.4990
G	 0.6580	 0.2290
H	 0.9220	 0.4710
I	 0.8980	 0.4460
J	 0.9350	 0.5100
K	 0.9560	 0.5150
L	 0.8930	 0.4450
N	 0.9210	 0.3470
P	 0.8790	 0.4100
T	 0.9070	 0.3940
U	 0.7320	 0.2420

