



wwPDB EM Validation Summary Report ⓘ

Jul 14, 2024 – 08:17 pm BST

PDB ID : 8AD1
EMDB ID : EMD-15357
Title : RNA polymerase at U-rich pause bound to RNA putL triple mutant - pause prone, closed clamp state
Authors : Dey, S.; Weixlbaumer, A.
Deposited on : 2022-07-07
Resolution : 4.10 Å(reported)
Based on initial model : 6ALH

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:

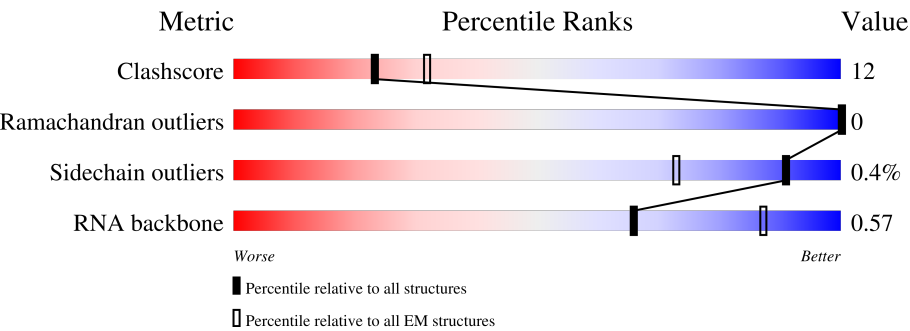
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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
RNA backbone	4643	859

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	N	266	<div><div></div><div>5% .</div><div>91%</div></div>
2	R	93	<div><div></div><div>9%</div><div>89%</div></div>
3	T	266	<div><div></div><div>5% 8%</div><div>86%</div></div>
4	E	91	<div><div>35%</div><div>54%</div><div>26%</div><div>20%</div></div>
5	F	613	<div><div>37%</div><div>23%</div><div>15%</div><div>61%</div></div>
6	A	329	<div><div></div><div>50%</div><div>18%</div><div>33%</div></div>
6	B	329	<div><div></div><div>47%</div><div>19%</div><div>34%</div></div>

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Mol	Chain	Length	Quality of chain
7	C	1342	<div><div></div><div>8%</div><div>71%</div><div>27%</div><div></div></div>
8	D	1406	<div><div></div><div>11%</div><div>67%</div><div>27%</div><div>5%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28169 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 DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	25	Total	C	N	O	P	0	0
			514	245	94	150	25		

- Molecule 2 is a RNA chain called RNA putL triple mutant.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	10	Total	C	N	O	P	0	0
			209	93	30	76	10		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	14	C	G	engineered mutation	GB 1877730557
R	37	U	A	engineered mutation	GB 1877730557
R	40	C	G	engineered mutation	GB 1877730557

- Molecule 3 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	36	Total	C	N	O	P	0	0
			739	351	141	211	36		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	73	Total	C	N	O	S	0	0
			582	355	111	115	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	237	Total	C	N	O	S	0	0
			1938	1223	347	356	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	571	HIS	TYR	conflict	UNP P00579

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	221	Total	C	N	O	S	0	0
			1706	1068	300	332	6		
6	B	218	Total	C	N	O	S	0	0
			1683	1051	297	329	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	1319	Total	C	N	O	S	0	0
			10407	6530	1814	2020	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	1335	Total	C	N	O	S	0	0
			10388	6526	1854	1958	50		

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

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

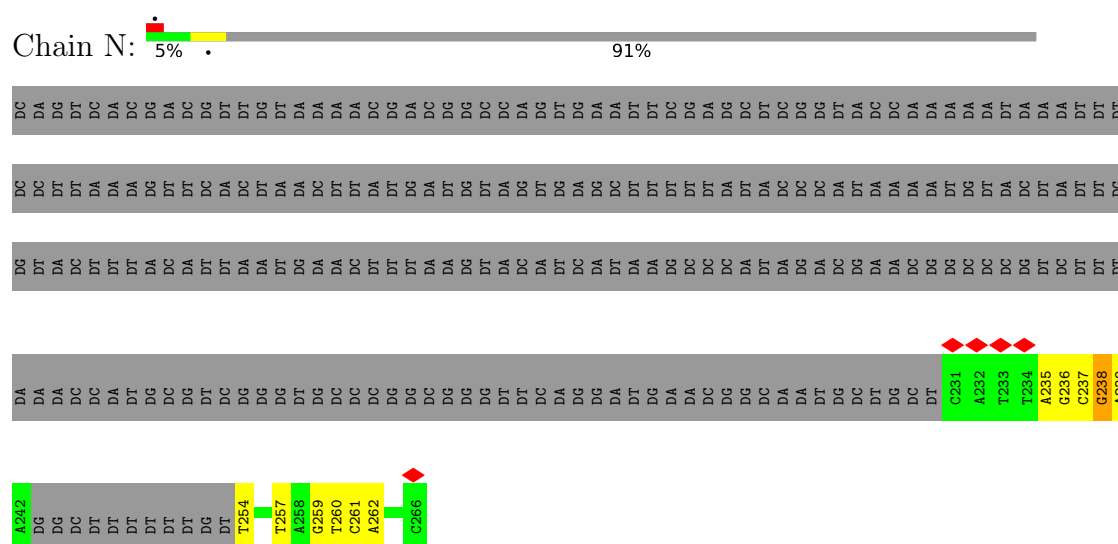
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

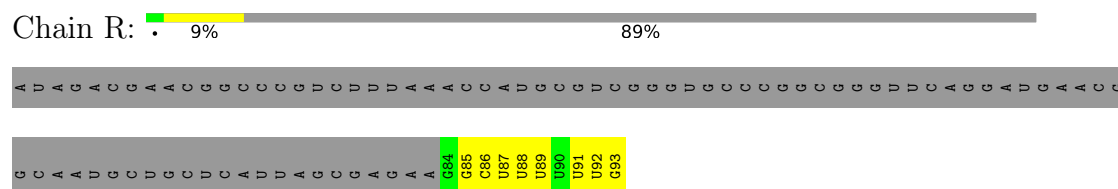
3 Residue-property plots [i](#)

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.

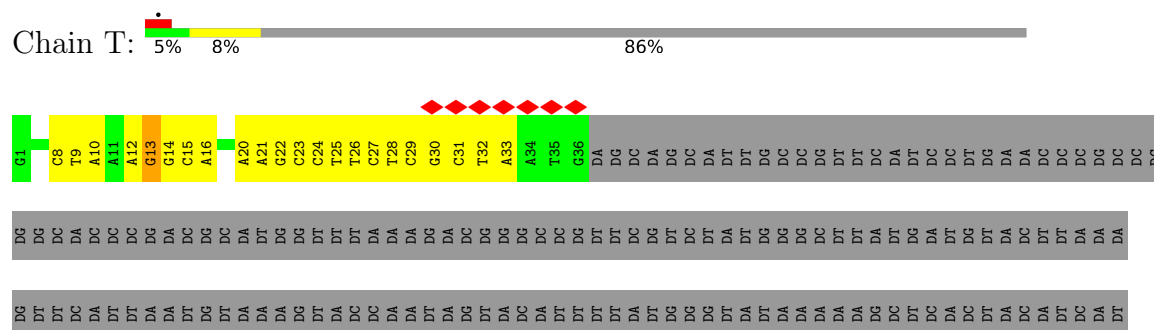
• Molecule 1: Non-template DNA



• Molecule 2: RNA putL triple mutant



• Molecule 3: Template DNA



- Molecule 4: DNA-directed RNA polymerase subunit omega

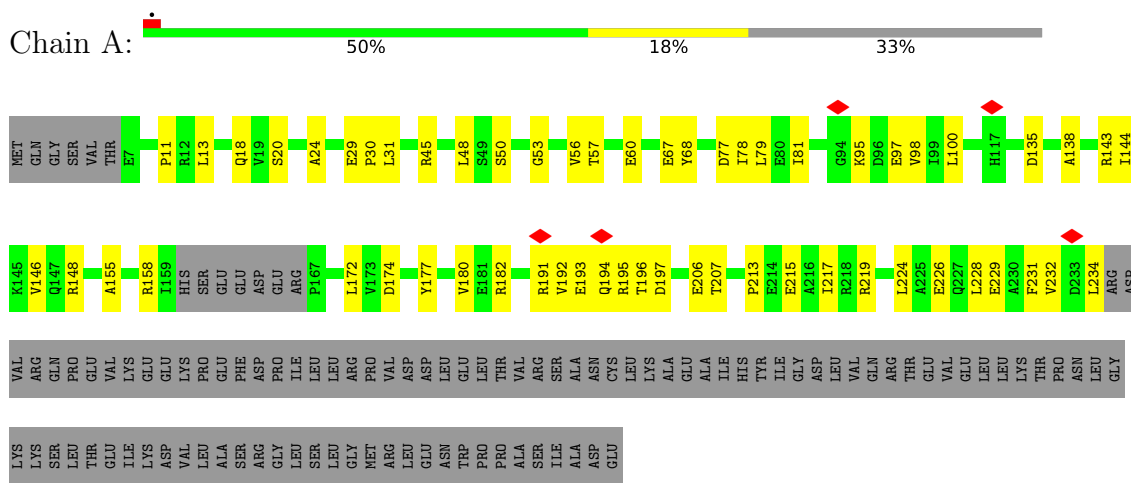
[illegible]

Chain F: 

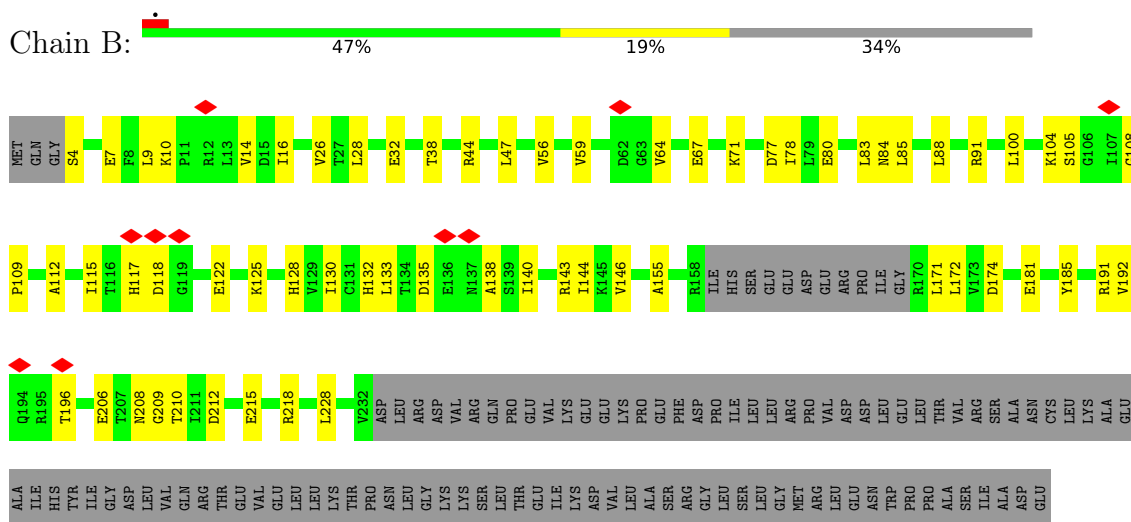
ARG	ALA	ALA	THR	HIS	ASP	VAL	SER	N301	I361	Y421	GLU
ALA	ALA	ALA	ALA	THR	ALA	GLU	HIS	F302	N362	R422	GLU
THR	ALA	ALA	ALA	ALA	ALA	LEU	A243	I303	R363	R423	LEU
HIS	GLN	GLU	GLU	GLU	GLU	GLU	T244	T304	R364	R424	GLU
ASP	ASP	ARG	ARG	ARG	ARG	ARG	A245	L305	M365	Y425	ARG
VAL	VAL	MET	MET	MET	MET	MET	Q246	F306	S366	K426	MET
LEU	LEU	LEU	LEU	LEU	LEU	LEU	Q247	T307	I367	F427	LEU
LEU	LEU	LEU	LEU	LEU	LEU	LEU	E248	G308	G368	A249	LEU
LEU	LEU	LEU	LEU	LEU	LEU	LEU	I249	N309	E369	T429	PRO
LEU	LEU	LEU	LEU	LEU	LEU	LEU	L250	E310	A370	T430	GLU
VAL	VAL	VAL	VAL	VAL	VAL	VAL	K251	T311	A371	Y430	LYS
VAL	VAL	VAL	VAL	VAL	VAL	VAL	L252	T312	K371	A431	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	S253	S312	A372	A432	ARG
LYS	LYS	LYS	LYS	LYS	LYS	LYS	D313	D313	R373	W433	LYS
VAL	VAL	VAL	VAL	VAL	VAL	VAL	E254	T314	R374	W434	VAL
LEU	LEU	LEU	LEU	LEU	LEU	LEU	V255	V315	A375	I435	LEU
LEU	LEU	LEU	LEU	LEU	LEU	LEU	F256	F316	K376	I436	LYS
MET	MET	MET	MET	MET	MET	MET	K257	N317	K377	Q437	ILE
ARG	ARG	ARG	ARG	ARG	ARG	ARG	Q258	A318	E378	A438	LYS
PHE	PHE	PHE	PHE	PHE	PHE	PHE	F259	A319	M379	I439	GLU
GLY	GLY	GLY	GLY	GLY	GLY	GLY	R260	T320	V380	I440	PRO
ILE	ILE	ILE	ILE	ILE	ILE	ILE	L261	I321	E381	T440	ILE
ASP	ASP	ASP	ASP	ASP	ASP	ASP	V262	A321	S382	R441	SER
ASP	ASP	ASP	ASP	ASP	ASP	ASP	P263	K322	A383	S442	MET
ASN	ASN	ASN	ASN	ASN	ASN	ASN	K264	N323	N383	I443	GLU
THR	THR	THR	THR	THR	THR	THR	Q265	K324	L384	A444	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	F266	F325	R385	D445	PRO
HIS	HIS	HIS	HIS	HIS	HIS	HIS	D267	V326	I386	GLN	ILE
LEU	LEU	LEU	LEU	LEU	LEU	LEU	S277	V327	V387	ASP	
LEU	LEU	LEU	LEU	LEU	LEU	LEU	Y268	E328	I388	ALA	
VAL	VAL	VAL	VAL	VAL	VAL	VAL	L269	F329	S389	ARG	
VAL	VAL	VAL	VAL	VAL	VAL	VAL	V270	L330	I390	THR	
GLY	GLY	GLY	GLY	GLY	GLY	GLY	N271	H331	A391	ILE	
ASP	ASP	ASP	ASP	ASP	ASP	ASP	E272	D332	K392	PRO	
ASP	ASP	ASP	ASP	ASP	ASP	ASP	S273	V333	S393	VAL	
VAL	VAL	VAL	VAL	VAL	VAL	VAL	R274	E334	T394	HIS	
THR	THR	THR	THR	THR	THR	THR	V275	S335	M395	ILE	
GLU	GLU	GLU	GLU	GLU	GLU	GLU	M276	E336	ASN	GLU	
ASP	ASP	ASP	ASP	ASP	ASP	ASP	M277	E337	ARG	THR	
THR	THR	THR	THR	THR	THR	THR	D278	V337	GLY	ILE	
LEU	LEU	LEU	LEU	LEU	LEU	LEU	R279	H338	LEU	THR	
GLN	GLN	GLN	GLN	GLN	GLN	GLN	V280	R339	GLN	ASN	
LEU	LEU	LEU	LEU	LEU	LEU	LEU	R281	A340	PHE	LEU	
ALA	ALA	ALA	ALA	ALA	ALA	ALA	T282	L341	L402	ASN	
LYS	LYS	LYS	LYS	LYS	LYS	LYS	Q283	Q342	D403	LEU	
ALA	ALA	ALA	ALA	ALA	ALA	ALA	E284	K343	L404	ARG	
LEU	LEU	LEU	LEU	LEU	LEU	LEU	R285	L344	I405	SER	
LYS	LYS	LYS	LYS	LYS	LYS	LYS	L286	Q345	Q406	ALA	
ARG	ARG	ARG	ARG	ARG	ARG	ARG	I287	Q346	E		

PRO
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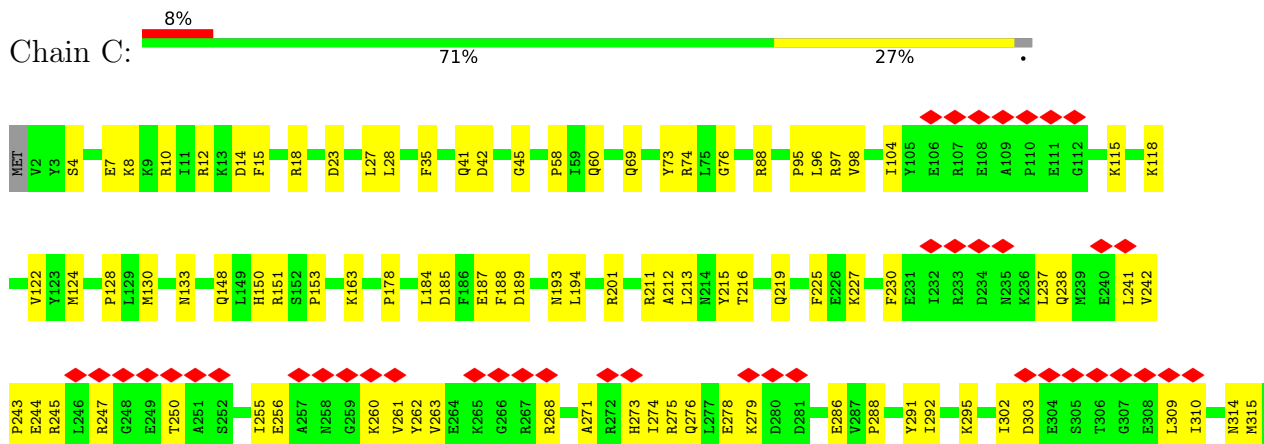
• Molecule 6: DNA-directed RNA polymerase subunit alpha

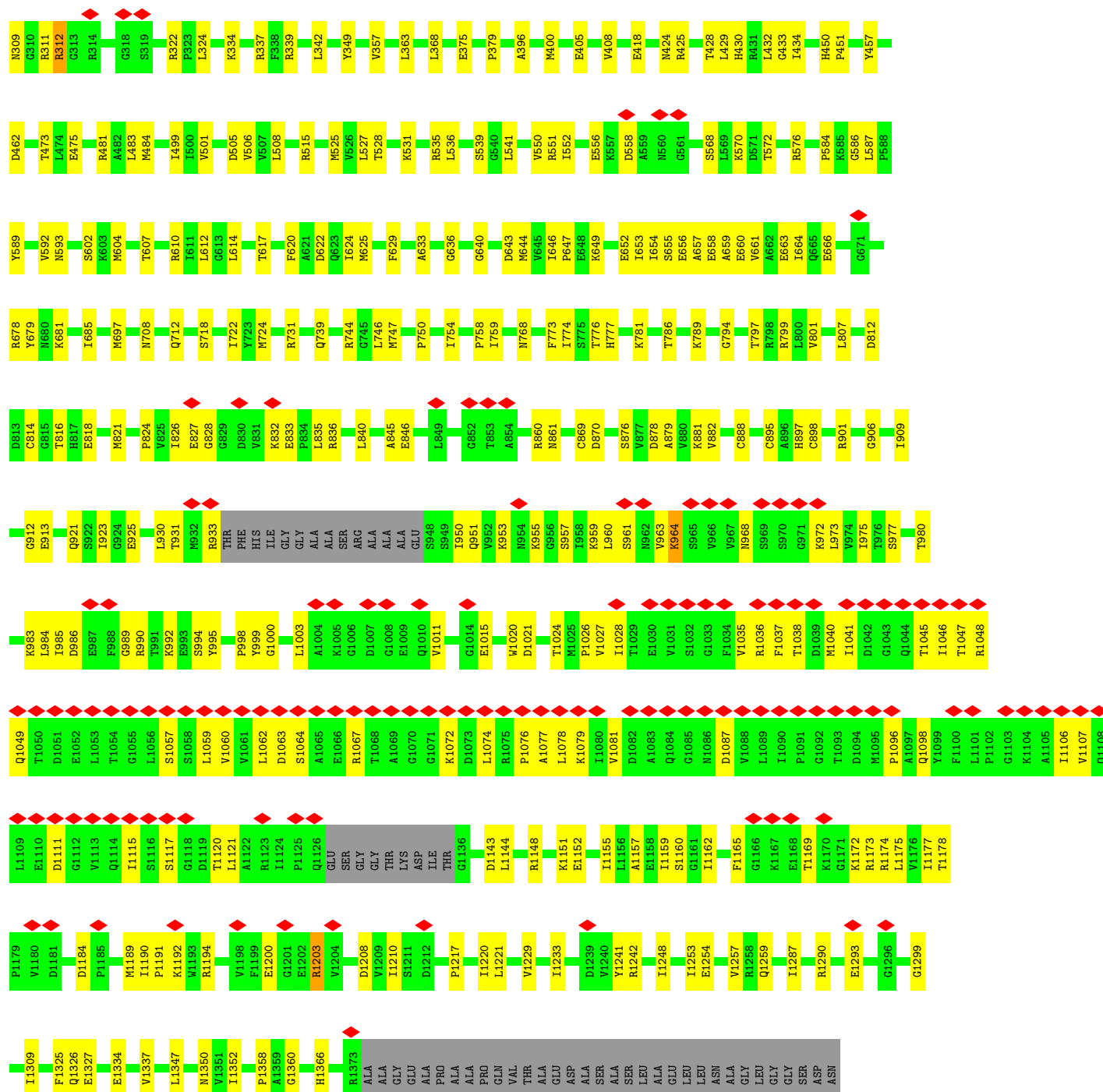


• Molecule 6: DNA-directed RNA polymerase subunit alpha



• Molecule 7: DNA-directed RNA polymerase subunit beta





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93293	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.436	Depositor
Minimum map value	-0.166	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.118	Depositor
Map size (\AA)	310.32, 310.32, 310.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.86200005, 0.86200005, 0.86200005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, IGU, 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	N	0.52	0/575	0.95	1/883 (0.1%)
2	R	0.26	0/231	0.89	0/357
3	T	0.52	0/779	0.86	0/1196
4	E	0.25	0/584	0.58	0/786
5	F	0.24	0/1961	0.50	0/2625
6	A	0.26	0/1726	0.55	1/2338 (0.0%)
6	B	0.25	0/1702	0.51	0/2306
7	C	0.26	0/10573	0.51	0/14265
8	D	0.25	0/10545	0.51	0/14236
All	All	0.27	0/28676	0.55	2/38992 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	238	DG	O4'-C4'-C3'	-5.13	102.45	104.50
6	A	50	SER	C-N-CA	5.11	134.47	121.70

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	N	514	0	284	7	0
2	R	209	0	104	7	0
3	T	739	0	404	14	0
4	E	582	0	593	18	0
5	F	1938	0	1992	76	0
6	A	1706	0	1746	41	0
6	B	1683	0	1719	41	0
7	C	10407	0	10420	253	0
8	D	10388	0	10611	271	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	28169	0	27873	690	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 12.

The worst 5 of 690 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)
8:D:888:CYS:HB2	8:D:898:CYS:SG	2.03	0.97
8:D:429:LEU:O	8:D:921:GLN:NE2	1.99	0.96
8:D:309:ASN:ND2	8:D:324:LEU:O	2.16	0.79
8:D:268:LEU:HD23	8:D:306:LEU:HA	1.64	0.79
7:C:968:GLU:HA	7:C:971:LEU:HG	1.67	0.76

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	
4	E	71/91 (78%)	69 (97%)	2 (3%)	0	100	100
5	F	229/613 (37%)	210 (92%)	19 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	217/329 (66%)	206 (95%)	11 (5%)	0	100	100
6	B	214/329 (65%)	208 (97%)	6 (3%)	0	100	100
7	C	1315/1342 (98%)	1264 (96%)	51 (4%)	0	100	100
8	D	1329/1406 (94%)	1276 (96%)	53 (4%)	0	100	100
All	All	3375/4110 (82%)	3233 (96%)	142 (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	
4	E	63/75 (84%)	63 (100%)	0	100	100
5	F	209/540 (39%)	206 (99%)	3 (1%)	67	80
6	A	189/286 (66%)	189 (100%)	0	100	100
6	B	187/286 (65%)	186 (100%)	1 (0%)	88	93
7	C	1138/1157 (98%)	1134 (100%)	4 (0%)	91	94
8	D	1120/1167 (96%)	1116 (100%)	4 (0%)	91	94
All	All	2906/3511 (83%)	2894 (100%)	12 (0%)	91	94

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	C	1106	ARG
8	D	87	LYS
8	D	1203	ARG
8	D	312	ARG
6	B	143	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
8	D	196	GLN
8	D	200	GLN
8	D	921	GLN
5	F	406	GLN
6	A	18	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	9/93 (9%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	85	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IGU	T	14	3	21,24,25	1.32	4 (19%)	30,35,38	2.03	10 (33%)
3	IGU	T	13	1,3	21,24,25	1.25	3 (14%)	30,35,38	1.72	6 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IGU	T	14	3	-	0/7/21/22	0/3/3/3
3	IGU	T	13	1,3	-	0/7/21/22	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	14	IGU	C5-C6	3.35	1.48	1.40
3	T	13	IGU	C5-C6	3.01	1.47	1.40
3	T	14	IGU	O3'-C3'	2.52	1.48	1.43
3	T	13	IGU	C5-N7	-2.40	1.34	1.39
3	T	13	IGU	C4-N9	-2.40	1.31	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	13	IGU	C6-C5-N7	4.95	136.31	130.21
3	T	14	IGU	C6-C5-N7	4.79	136.11	130.21
3	T	14	IGU	O4'-C1'-N9	4.09	115.17	107.86
3	T	14	IGU	C2'-C1'-N9	-4.02	104.52	113.77
3	T	14	IGU	C5-C4-N3	-3.48	119.62	127.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	13	IGU	1	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

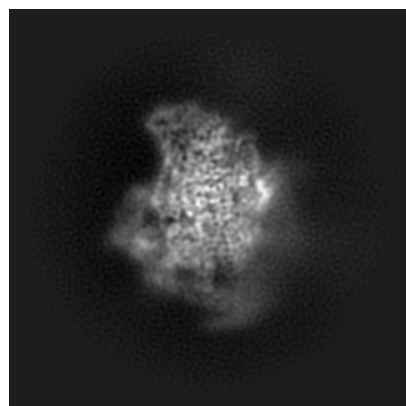
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15357. These allow visual inspection of the internal detail of the map and identification of artifacts.

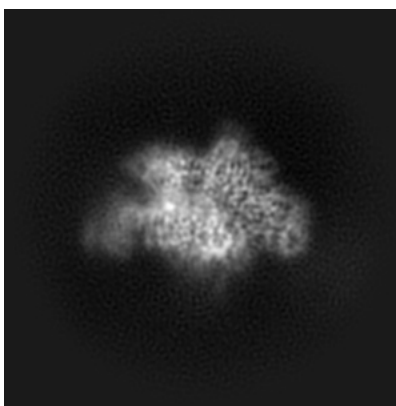
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

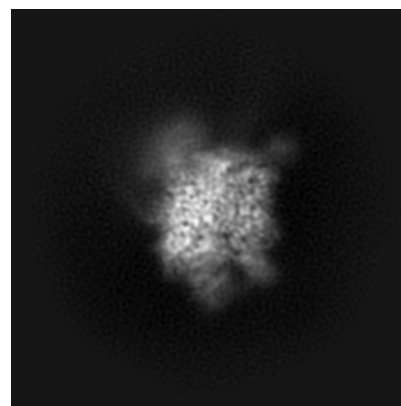
6.1.1 Primary map



X

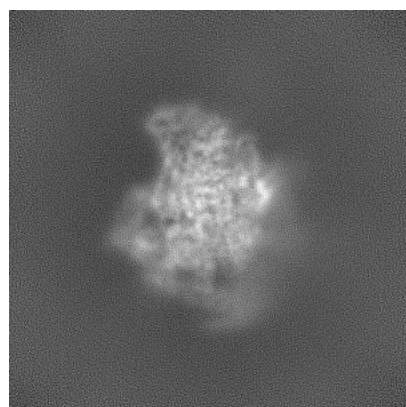


Y

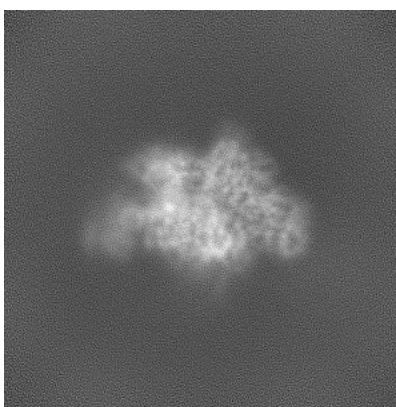


Z

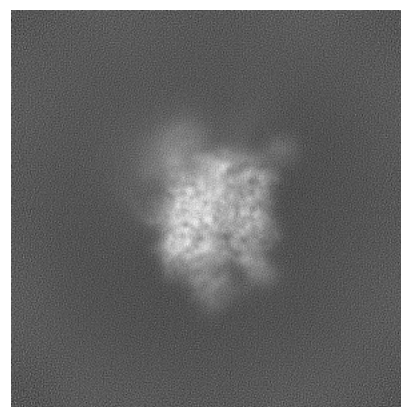
6.1.2 Raw map



X



Y

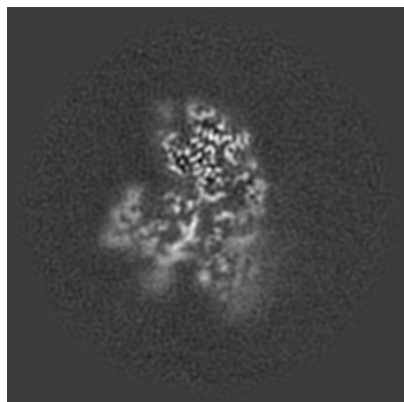


Z

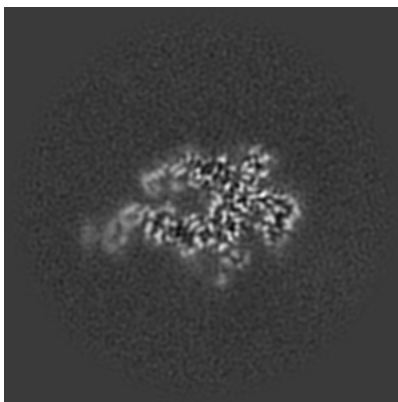
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

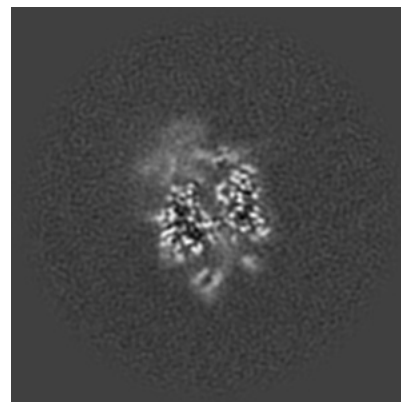
6.2.1 Primary map



X Index: 180

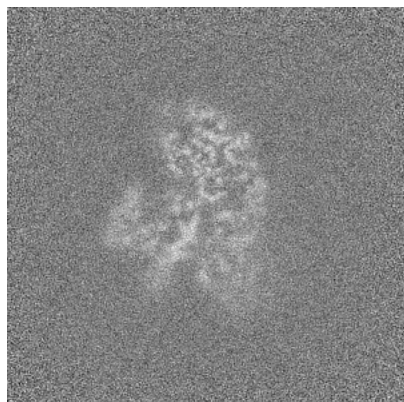


Y Index: 180

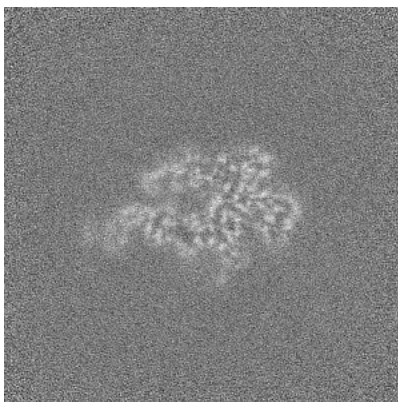


Z Index: 180

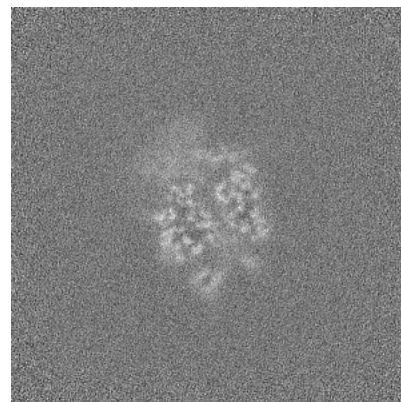
6.2.2 Raw map



X Index: 180



Y Index: 180

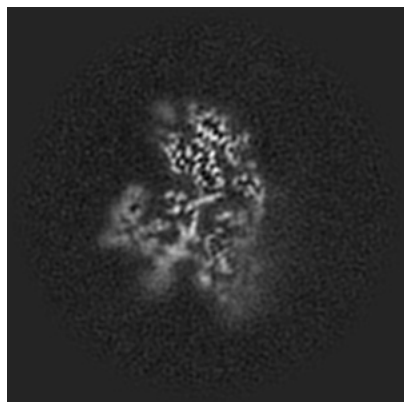


Z Index: 180

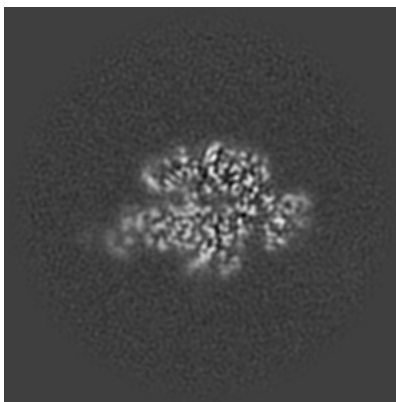
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

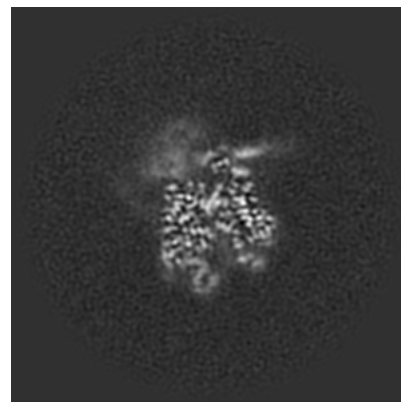
6.3.1 Primary map



X Index: 178

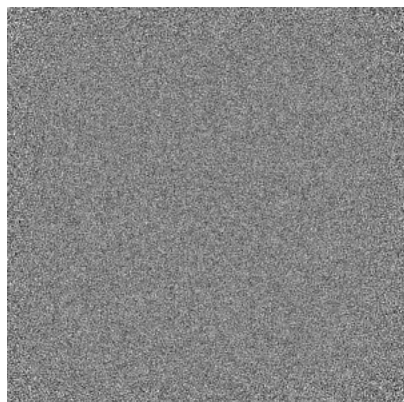


Y Index: 170

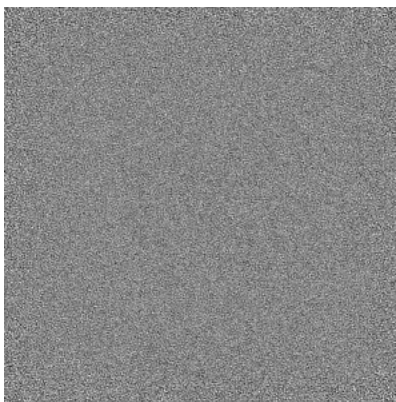


Z Index: 187

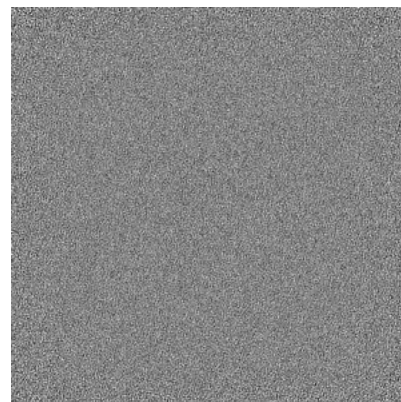
6.3.2 Raw map



X Index: 0



Y Index: 0

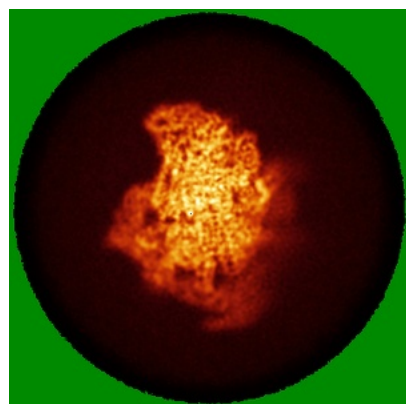


Z Index: 0

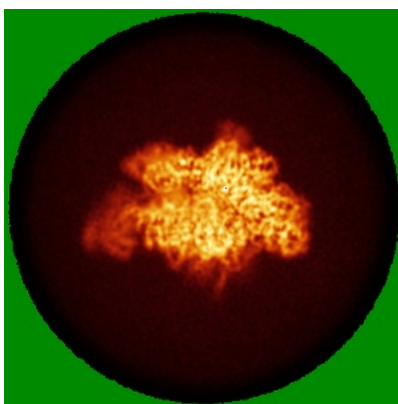
The images above show the largest variance slices of the map in three orthogonal directions.

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

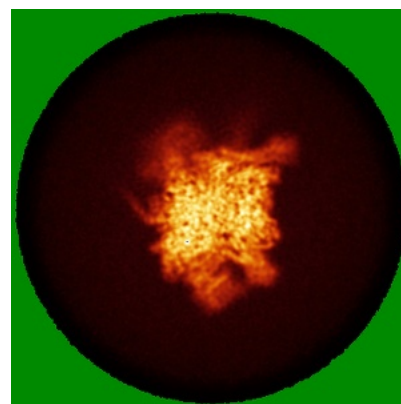
6.4.1 Primary map



X

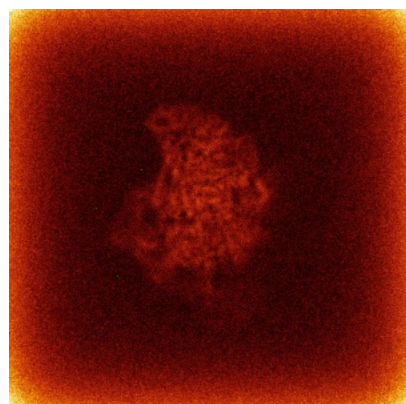


Y

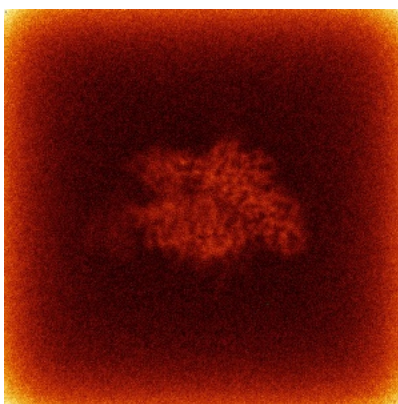


Z

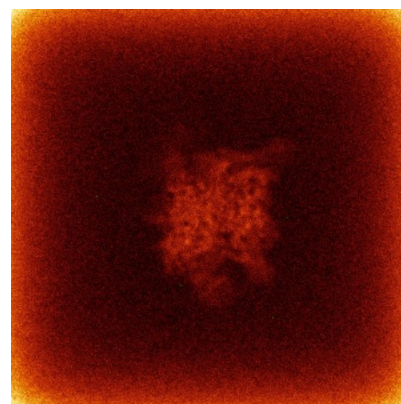
6.4.2 Raw map



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.

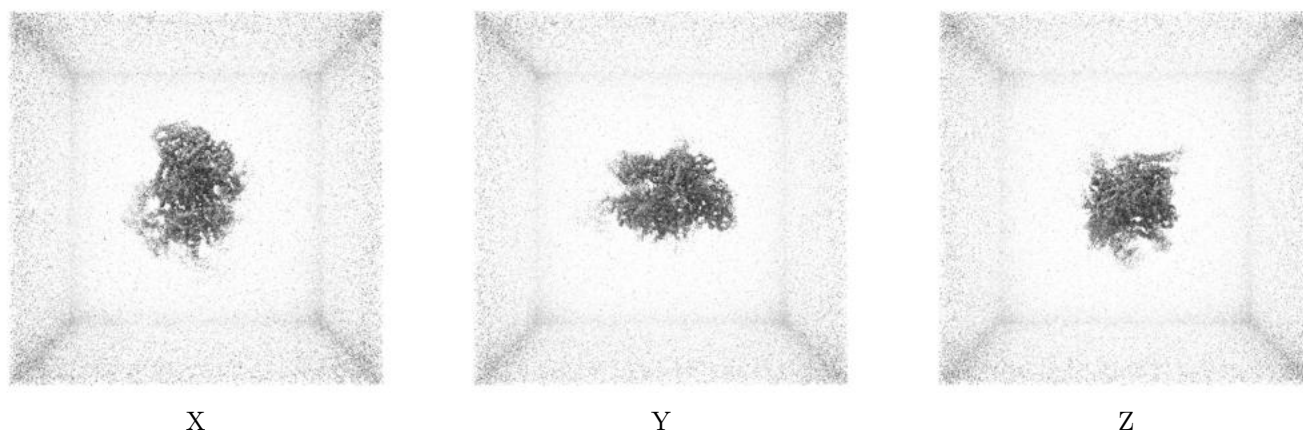
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.118. 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.

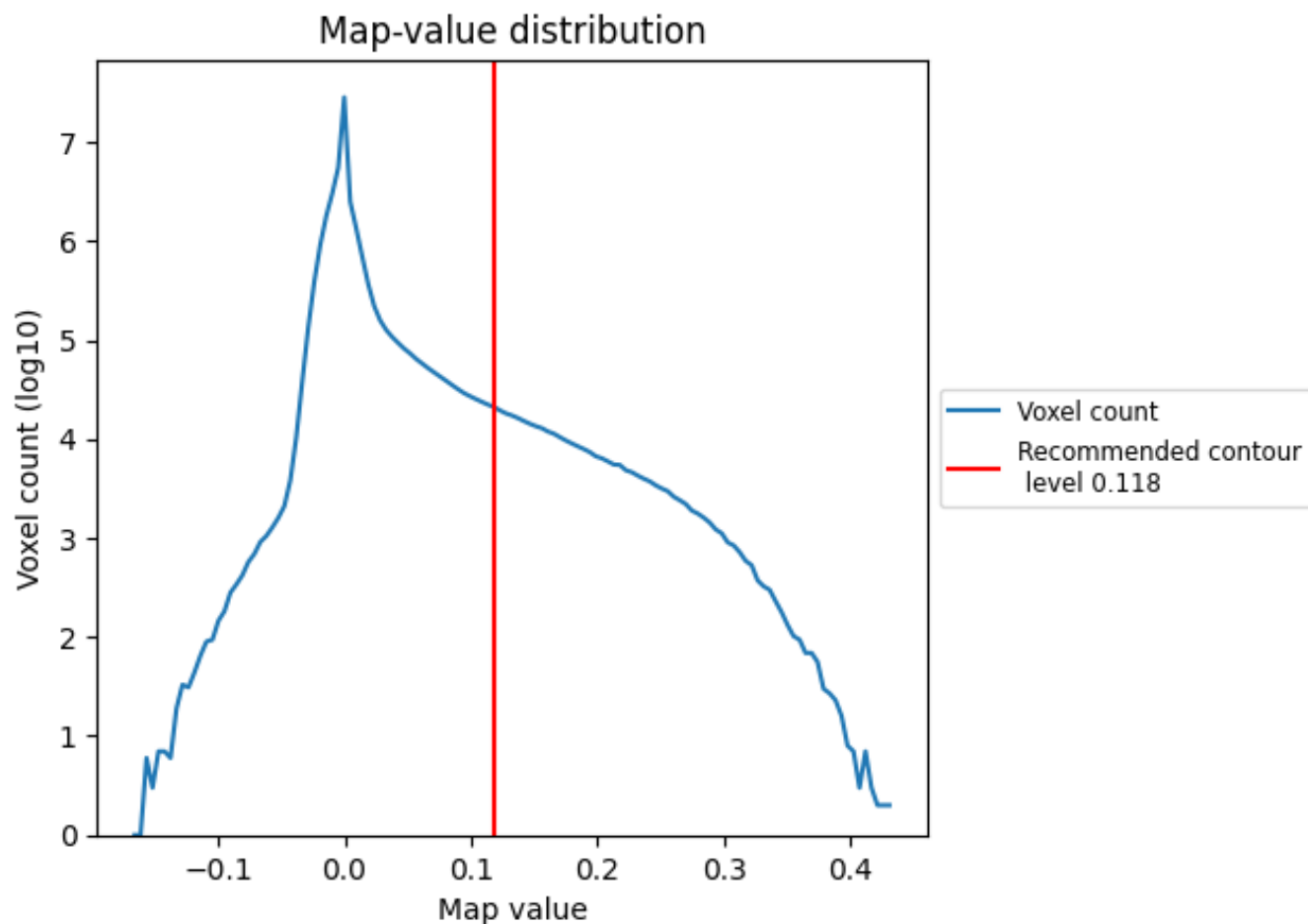
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

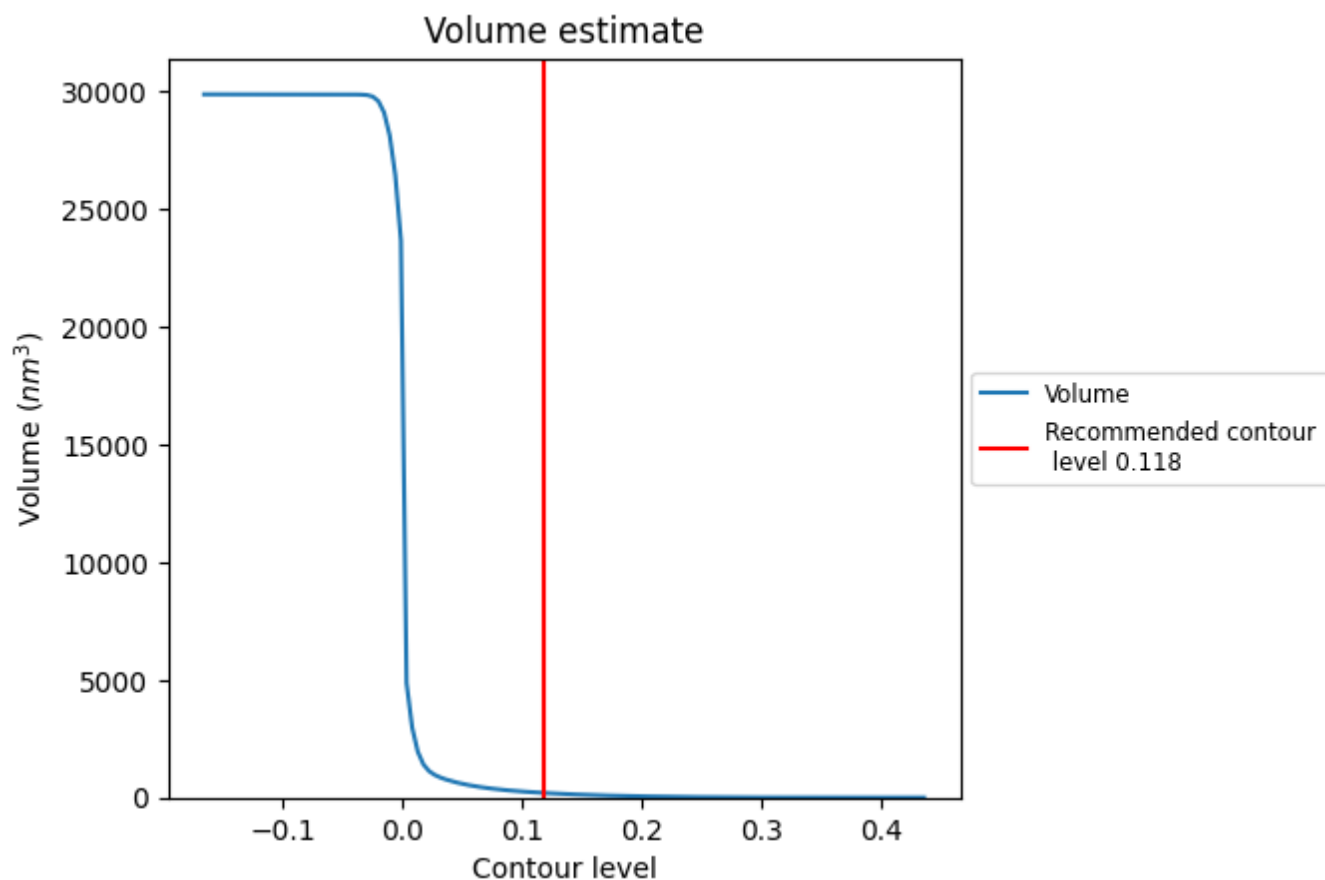
This section contains the results of statistical analysis of the map.

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.

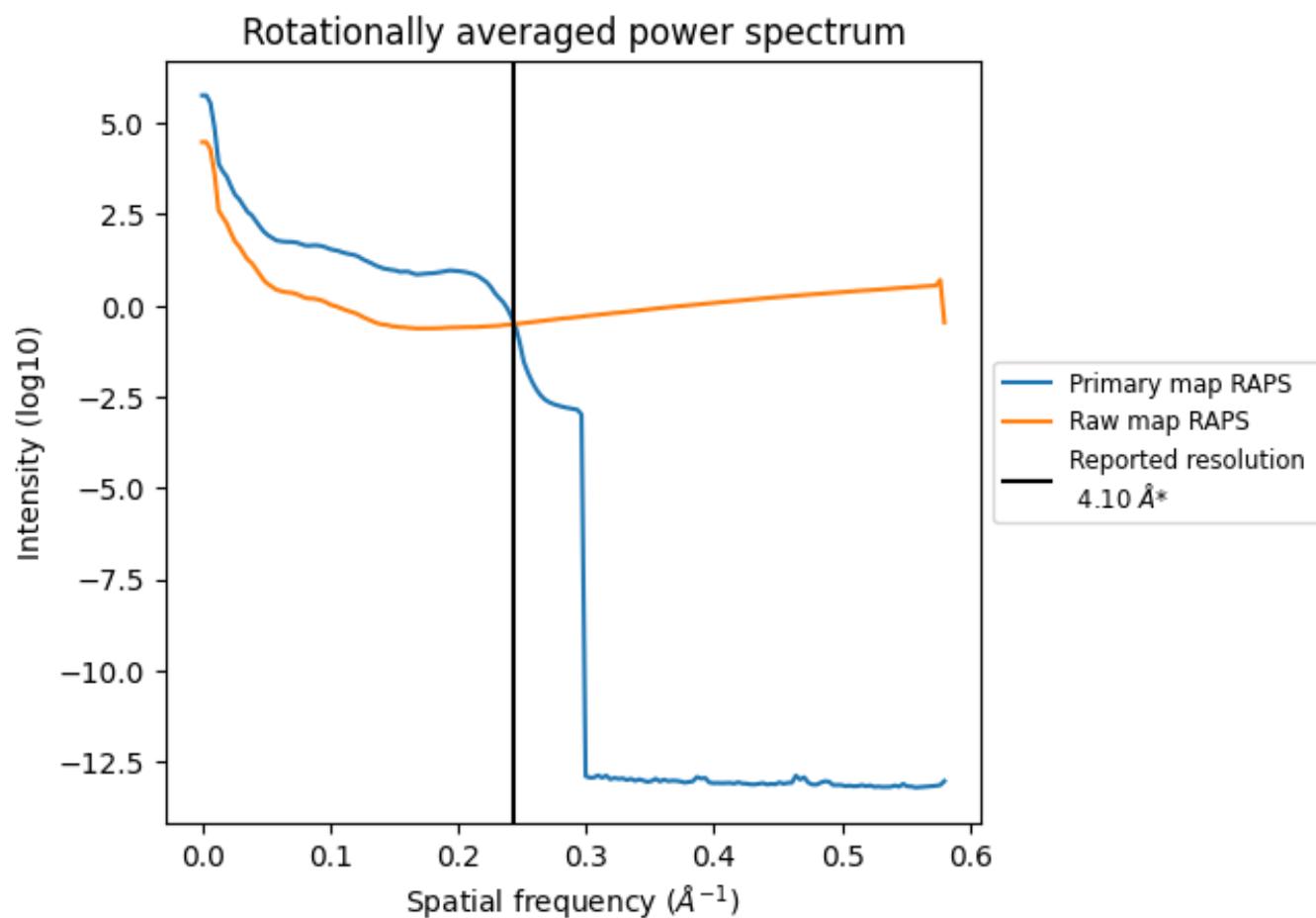
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm³; this corresponds to an approximate mass of 178 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 ⓘ

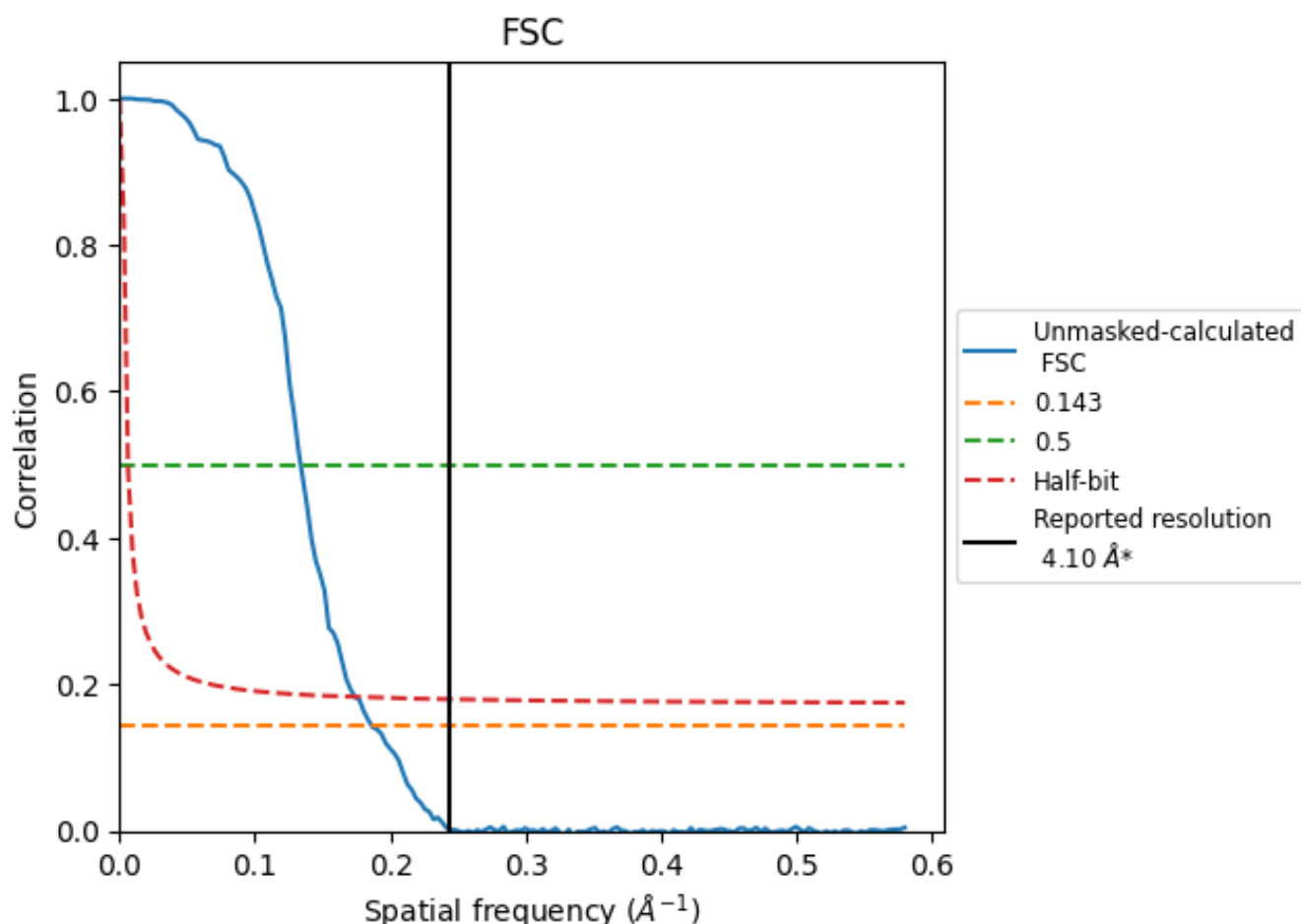


*Reported resolution corresponds to spatial frequency of 0.244 \AA^{-1}

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

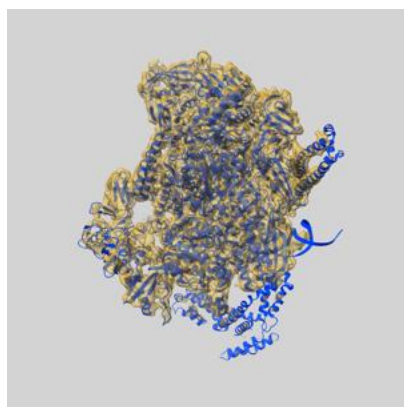
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.36	7.47	5.75

*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 5.36 differs from the reported value 4.1 by more than 10 %

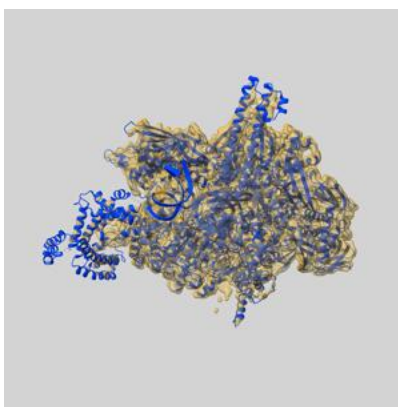
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15357 and PDB model 8AD1. Per-residue inclusion information can be found in section [3](#) on page [6](#).

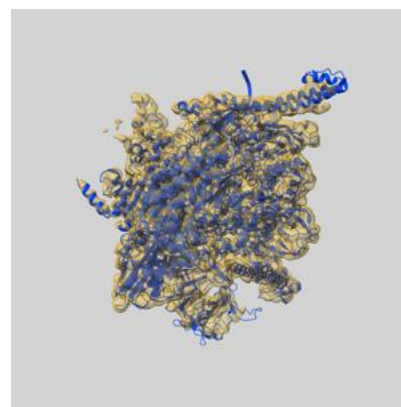
9.1 Map-model overlay [i](#)



X



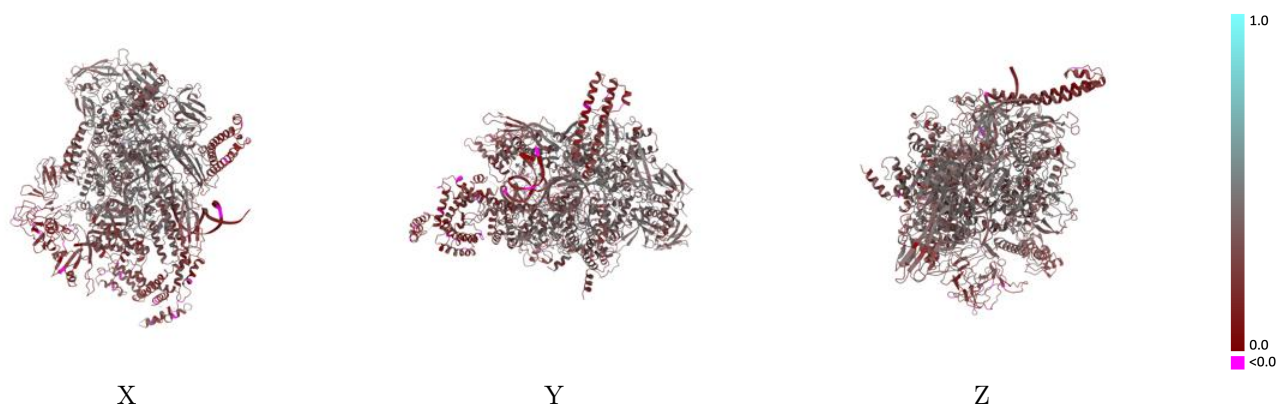
Y



Z

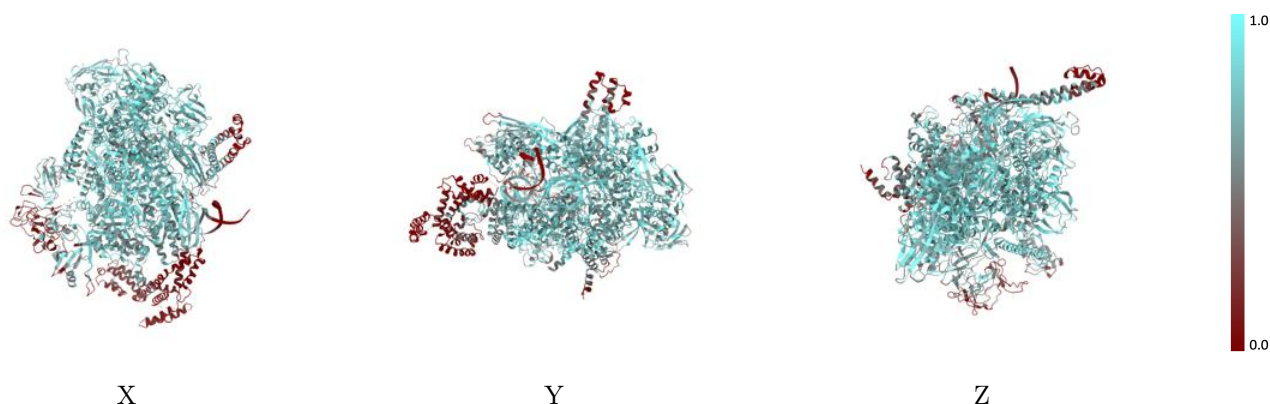
The images above show the 3D surface view of the map at the recommended contour level 0.118 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



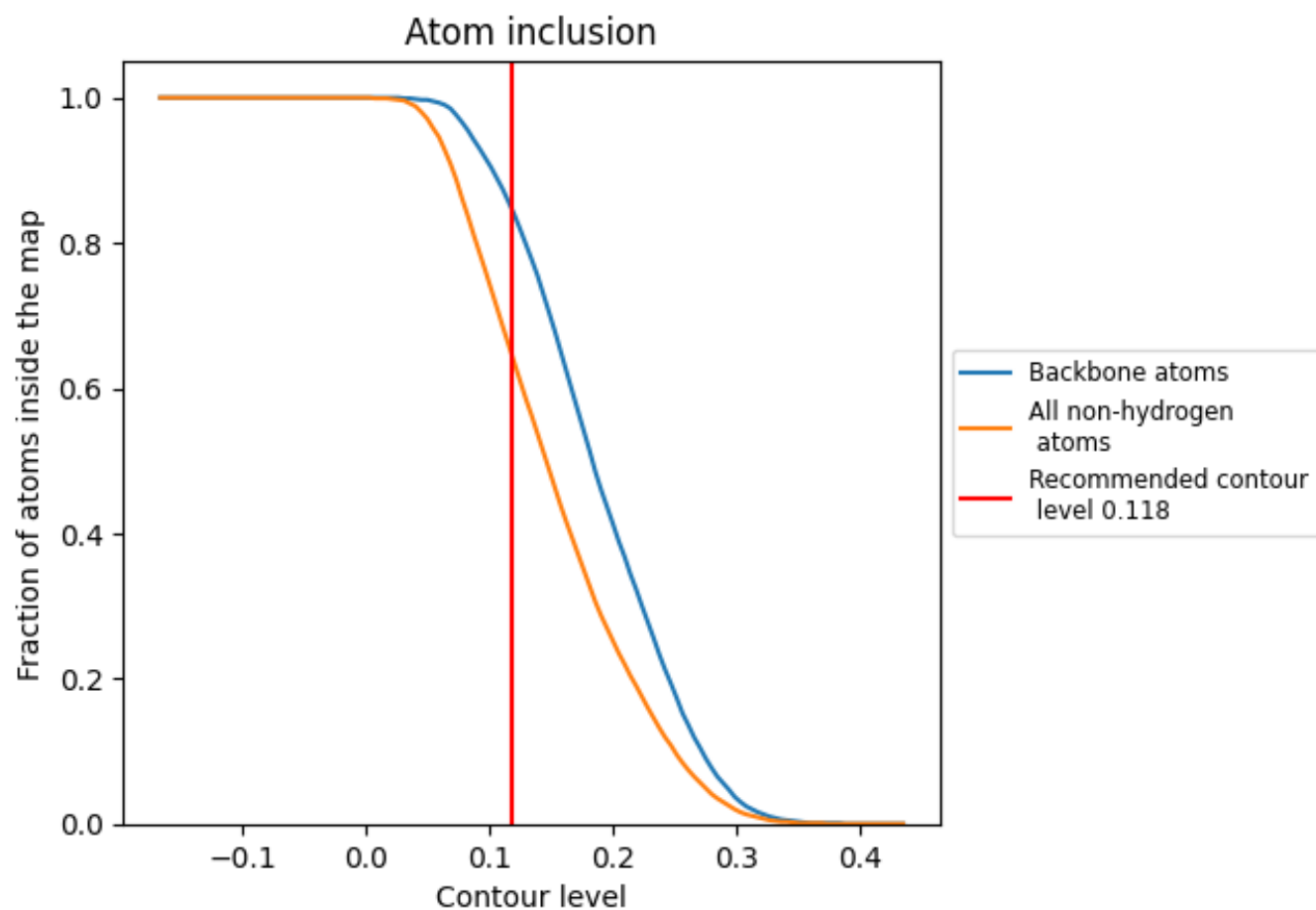
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.118).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 65% 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 (0.118) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6490	<div></div> 0.3370
A	<div></div> 0.7510	<div></div> 0.3920
B	<div></div> 0.7290	<div></div> 0.3720
C	<div></div> 0.7020	<div></div> 0.3550
D	<div></div> 0.6800	<div></div> 0.3420
E	<div></div> 0.4010	<div></div> 0.3150
F	<div></div> 0.0680	<div></div> 0.1950
N	<div></div> 0.6070	<div></div> 0.2110
R	<div></div> 0.9040	<div></div> 0.3780
T	<div></div> 0.7020	<div></div> 0.2590

