



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 04:40 PM EST

PDB ID : 8H40
EMDB ID : EMD-34476
Title : Cryo-EM structure of the transcription activation complex NtcA-TAC
Authors : Han, S.J.; Jiang, Y.L.; You, L.L.; Shen, L.Q.; Wu, X.X.; Yang, F.; Kong, W.W.; Chen, Z.P.; Zhang, Y.; Zhou, C.Z.
Deposited on : 2022-10-09
Resolution : 3.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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:

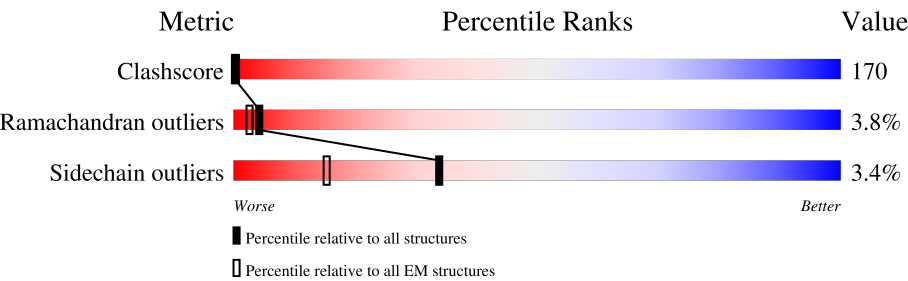
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.60 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

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	1	125	<div><div></div><div>48%</div><div></div><div>47%</div></div>
2	2	125	<div><div>7%</div><div>35%</div><div></div><div>57%</div></div>
3	A	1132	<div><div>10%</div><div>41%</div><div>42%</div><div>5%</div></div>
4	B	1350	<div><div>8%</div><div>54%</div><div>26%</div><div>10%</div></div>
5	C	236	<div><div>5%</div><div>7%</div><div>49%</div><div>37%</div><div></div></div>
5	D	236	<div><div>9%</div><div>5%</div><div>49%</div><div>39%</div><div></div></div>
6	E	625	<div><div>11%</div><div>46%</div><div>40%</div><div></div></div>
7	F	78	<div><div>6%</div><div>21%</div><div>36%</div><div>17%</div><div>26%</div></div>

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Mol	Chain	Length	Quality of chain
8	G	390	
9	X	223	
9	Y	223	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 34833 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 DNA (125-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	66	Total	C	N	O	P	0	0
			1358	651	243	398	66		

- Molecule 2 is a DNA chain called DNA (125-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	54	Total	C	N	O	P	0	0
			1109	532	203	320	54		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1077	Total	C	N	O	S	0	0
			8473	5326	1505	1618	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P22703
A	1	VAL	-	expression tag	UNP P22703

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	1217	Total	C	N	O	S	0	0
			9292	5802	1639	1823	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	226	Total	C	N	O	S	0	0
			1762	1106	305	346	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	226	Total	C	N	O	S	0	0
			1762	1106	305	346	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP Q8YPK3
C	1	VAL	-	expression tag	UNP Q8YPK3
D	0	MET	-	initiating methionine	UNP Q8YPK3
D	1	VAL	-	expression tag	UNP Q8YPK3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	620	Total	C	N	O	S	0	0
			4923	3107	885	910	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	58	Total	C	N	O	S	0	0
			474	290	90	90	4		

- Molecule 8 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	314	Total	C	N	O	S	0	0
			2600	1628	482	484	6		

- Molecule 9 is a protein called NtcA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	196	Total	C	N	O	S	0	0
			1540	984	268	280	8		
9	Y	196	Total	C	N	O	S	0	0
			1540	984	268	280	8		

L1034	L1035	E1036	L1037	L1038	L1039	V1040	K1041	S1042	D1043	D1044	L1045	Q1046	G1047	R1048	L1049	E1050	A1051	L1052	L1053	A1054	L1055	V1056	K1057	G1058	K1059	A1060	I1061	P1062	G1065	T1066	P1067	E1068	S1069	T1070	G1008	K1071	V1072	L1073	M1074	R1075	E1076	L1077	Q1078	S1079	L1080	V1081	L1082	D1083	I1084	A1085	V1086	L1087	K1088	V1089	E1090	T1091	A1092	A1093	Y1032	D1094			
T973	I974	G975	V976	A977	L978	M979	L980	K981	L982	V983	H984	L985	V986	D987	R988	K989	L990	H991	A992	R993	S994	T995	G996	P997	X998	S999	L1000	V1001	T1002	Q1003	Q1004	P1005	G944	S1069	G1007	G1008	K1009	L1010	Q1011	Q1012	G1013	Q1015	R1016	F1017	G1018	E1021	V1022	W1023	A1024	L1025	G1026	A1027	F1028	G1029	A1030	Q1032	T1033						
G911	V912	R913	F914	K915	I916	T917	P918	F919	M922	Y923	G924	E925	E926	S927	S928	R929	R930	I931	V932	H933	G934	K935	L936	Q937	E938	A939	R940	D941	E942	T943	G944	K945	D946	V947	V948	Y949	N950	P951	D952	D953	K956	I957	M958	V959	Y960	D961	G962	R963	T964	G965	E966	A967	F968	D969	R970	P971	V972						
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K504	L505	P506	V507	A508	L509	K510	S511	D512	R513	E514	L515	G516	H517	I518	M519	N520	O521	P522	Q523	R524	S525	T526	U527	V528	W529	X530	Y531	Z532	A533	B534	C535	D536	E537	F538	G539	H540	I541	J542	K543	L544	M545	N546	O547	P548	Q549	R550	S551	T552	U553	V554	W555	X556	Y557	Z558									
L242	R243	P247	P248	T249	V250	L251	G252	K253	Q254	Q255	L256	L257	D258	R259	F260	R261	F262	D263	P264	K265	R266	Y267	D268	L269	G270	R271	N334	V272	G273	E208	R274	R275	L276	K277	L278	N279	L280	L281	R282	L283	S284	V285	D286	I287	T288	V289	R290	V291	L292	T293	S294	D295	L296	D297	T360	L298	A299	A300	V301	S302	Y303		
L304	L305	N306	P367	L307	E308	L309	D310	L311	G312	S313	D318	H319	L320	D321	N322	R323	R324	R325	R326	S327	V328	G329	R330	L331	L332	Q333	A334	Q335	Q336	R337	R338	R339	K399	L340	N341	R342	L343	E344	R345	I346	I347	R348	E349	M350	R351	V352	V353	S354	S355	A356	E357	V358	L359	M420	D421	T360	P361	A362	S363	A300	V301	S302	Y303
P367	K368	P369	V370	A371	A372	A373	I374	K375	S376	E377	F378	F379	S380	L381	G382	L443	L444	L445	L446	L447	F386	M387	D388	Q389	R390	T390	L391	P392	L393	L394	L395	G396	H397	L398	L399	L400	L401	L402	L403	L404	L405	E467	N468	G469	R470	V471	R472	F473	D474	Q475	P476	A477	Y478	M480	T481	I482	A483	E484	L485	E486	D487		
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D548	D549	N550	R551	R552	A553	L554	M555	G556	S557	N558	M559	Q560	R561	Q562	A563	V564	P565	L566	Q567	K568	P569	E570	R571	P572	L573	V574	G575	T576	G577	L578	E579	A580	Q581	G582	A583	R584	D585	S586	G587	M588	V589	I590	P591	S592	T593	D594	D595	G596	D597	V588	V599	Y600	V601	D602	A603	T604	E605	I606	R607				
V608	R609	V610	S611	G612	Q613	L614	P615	T616	A617	S618	Q619	K620	S621	T622	D623	N624	G625	Q626	R627	T628	S629	Q630	K631	G632	Q633	E634	R635	R636	T637	T638	V639	S640	K641	Y642	Q643	R644	S645	N646	Q647	D648	T649	C650	L651	N652	Q653	K654	P655	L656	V657	R658	T659	I660	R661	R662	V663	A665	G666	Q667					
V668	L669	A670	D671	G672	S673	S674	T675	E676	G677	R678	E679	L680	A681	L682	G683	Q684	N685	L686	V687	V688	A689	Y690	M691	P692	M693	E694	G695	V696	N697	Y698	E699	D700	A701	I702	L703	I704	S705	E706	R707	L708	V709	Q710	D711	D712	I713	T714	T715	T716	I717	H718	I719	E720	K721	Y722	R723	I724	E725	A726	R727				
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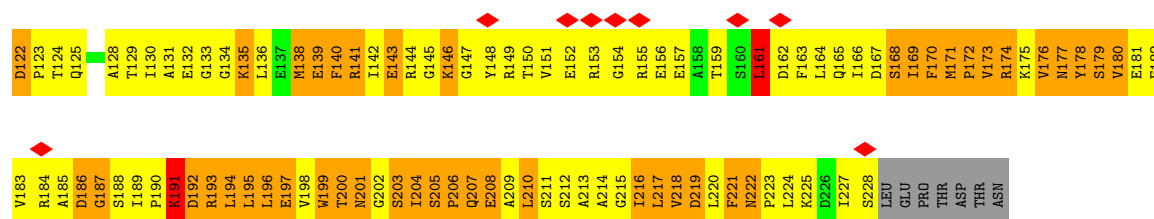
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ARG
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● Molecule 4: DNA-directed RNA polymerase subunit beta'

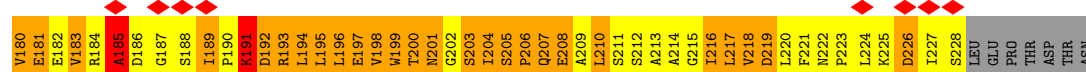
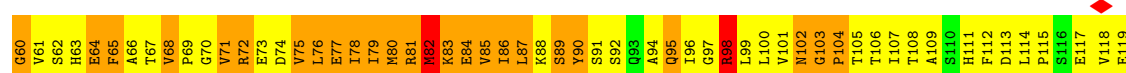
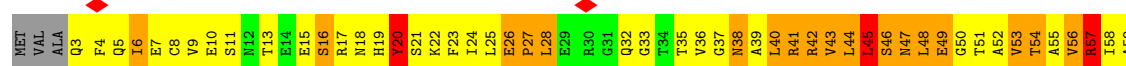


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N668	G608	Q548	Y488	V427	T367	K308	V248	T186	M125	S64
S669	V609	A549	N489	A428	H368	V309	H250	L187	A126	L65
G670	E610	T550	L490	L429	R369	D310	P251	L188	A127	L66
V671	G611	V551	P491	GLY	T370	L311	T251	R189	S128	E67
V672	Q612	T552	P492	GLY	R371	G312	K253	T190	R131	A68
E673	K613	V553	G493	ARG	H372	E313	T253	A191	G132	E70
V674	K614	Q554	A494	THR	G373	A314	K254	D192	M133	E71
T675	G615	S555	E495	THR	E374	V315	E255	S193	I134	E72
Q676	K616	S555	L496	THR	D375	G316	V256	G194	S135	I73
K677	K617	S556	V497	THR	A376	I317	T257	Y195	Q136	R74
N678	A617	V498	V497	THR	L377	A319	A258	L196	V137	A75
D679	K618	Q557	V498	T438	F378	A320	R260	R198	R138	T76
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L681	L619	R559	N500	T439	F378	A319	R262	L200	L140	E77
R682	G620	N560	G501	K440	V379	A320	T263	V201	L141	Q81
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V684	E622	Y562	R503	V442	E380	I323	T263	D202	Q142	Q81
V685	V623	L563	V504	K443	S381	G324	T264	D203	M147	Y81
V686	V624	I564	E505	D444	N382	E325	S265	G205	G145	R82
K687	Q625	T565	T506	V445	G383	G327	S265	Q205	L146	R82
P688	G626	T566	N507	A446	I384	T328	D267	D206	R144	T22
E689	G627	G567	G508	D448	K385	T328	L288	V207	G145	E84
T628	T628	N568	V509	L449	I386	Q329	A269	K270	M147	T85
L629	L629	N569	L510	A450	L387	T331	E271	I209	A148	T86
L630	L630	Q570	A511	G451	L387	K332	I272	R210	D149	E87
W631	W631	V571	E512	E452	E388	ARG	E273	E211	P150	V88
L632	L632	F572	T513	V453	P389	THR	K274	I212	Q151	E89
P633	P633	N573	K514	K454	R390	PHE	A275	D213	G152	R90
E634	E634	L574	L515	F455	K391	HIS	G276	C214	E153	T29
D695	D695	R575	T516	A456	E392	THR	V277	G215	E154	V31
T636	T636	A576	T517	E457	E392	GLY	A278	T216	I155	K33
H637	H637	T577	I518	V458	G393	GLY	E279	T220	D156	V94
E638	E638	P578	H519	V459	S394	VAL	V280	P221	L157	I95
V639	V639	G579	G520	P460	E395	PHE	V281	V222	D96	D34
N640	N640	K641	G521	E461	T396	THR	V282	R223	L157	K35
D642	D642	T580	V522	Q462	P397	GLY	R283	P224	P158	L36
I643	I643	K581	V523	K463	P397	GLY	S284	G160	I159	T37
S644	S644	V582	V523	R463	P397	VAL	P285	T161	K160	W98
Q583	Q583	R524	R524	T464	P399	ALA	L286	M225	G100	L39
L645	L645	L525	L525	D465	P399	ALA	T287	T226	T101	G40
L646	L646	P526	P526	R466	Q400	Q347	C288	E227	S102	S12
L647	L647	Q586	E527	Q467	E401	Q348	E289	G228	E103	F41
V648	V648	V587	A528	G468	I402	V349	A290	G166	A104	Y43
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D650	D650	A589	T529	T470	L403	S351	R291	T168	K106	T45
G651	G651	E590	P530	T471	V404	K352	R292	V169	D107	R46
Q652	Q652	L591	G531	T472	T405	K353	S293	T170	E108	A47
Y653	Y653	F532	K532	T473	Q406	R353	V294	E171	V109	G48
V654	V654	E533	S533	A474	Q407	D354	C295	Y172	V110	V49
E655	E655	T534	T534	A475	G407	C355	H297	I173	T111	S50
A656	A656	R595	E535	R476	S408	T356	Y299	I174	H112	I51
G657	G657	E536	E536	R476	T409	I357	C300	T237	S52	S52
T658	T658	I537	I537	R476	T409	K358	G300	S176	F113	V53
E659	E659	R597	E537	G477	L410	K358	K301	L239	K114	
V660	V660	Y596	E538	G478	Y411	L358	G301	L240	Y177	L56
V661	V661	T598	E538	L479	Y411	L359	H301	G241	G178	M117
K662	K662	T600	V540	L480	L412	P360	S302	R242	A179	P118
D663	D663	G601	T541	I481	V413	R361	L303	V243	R180	V58
G602	G602	A542	A542	I482	V413	R361	L303	V244	N120	P59
I664	I664	E642	E642	I482	D414	K362	L363	G245	K181	P60
T665	T665	L483	S543	L483	Q415	L363	R364		S121	
		S484	V544	S484	Q416	L363	R364		G182	
		V544	V544	G485	Q417	T365	H305		L183	
		K605	V545		Q417	T365	H305			
					V418					
					K419					
					K420					
					Q421					
					Q422					
					L423					
					L424					
					M425					
						</				

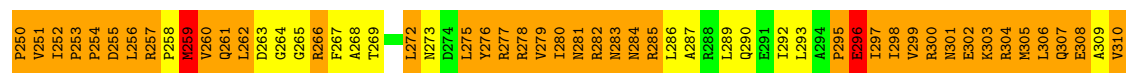
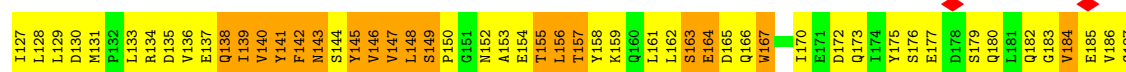


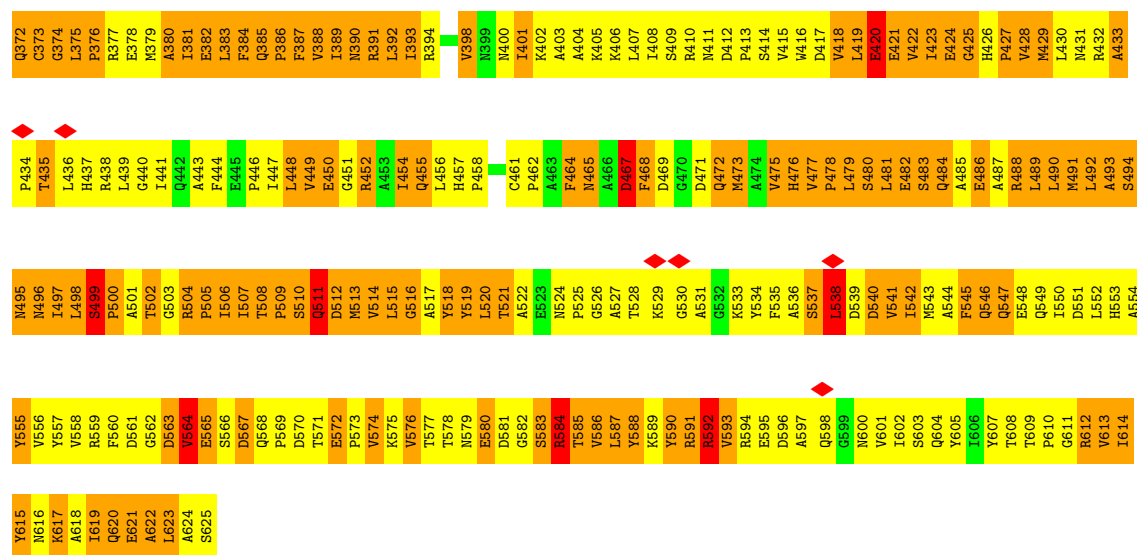


• Molecule 5: DNA-directed RNA polymerase subunit alpha

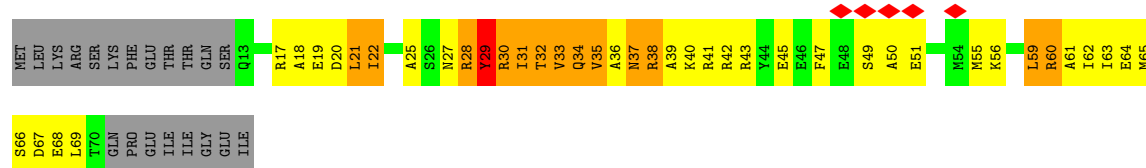
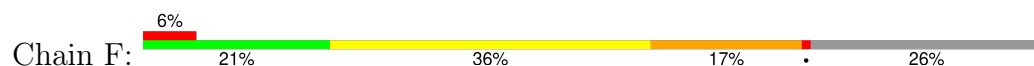


• Molecule 6: DNA-directed RNA polymerase subunit gamma

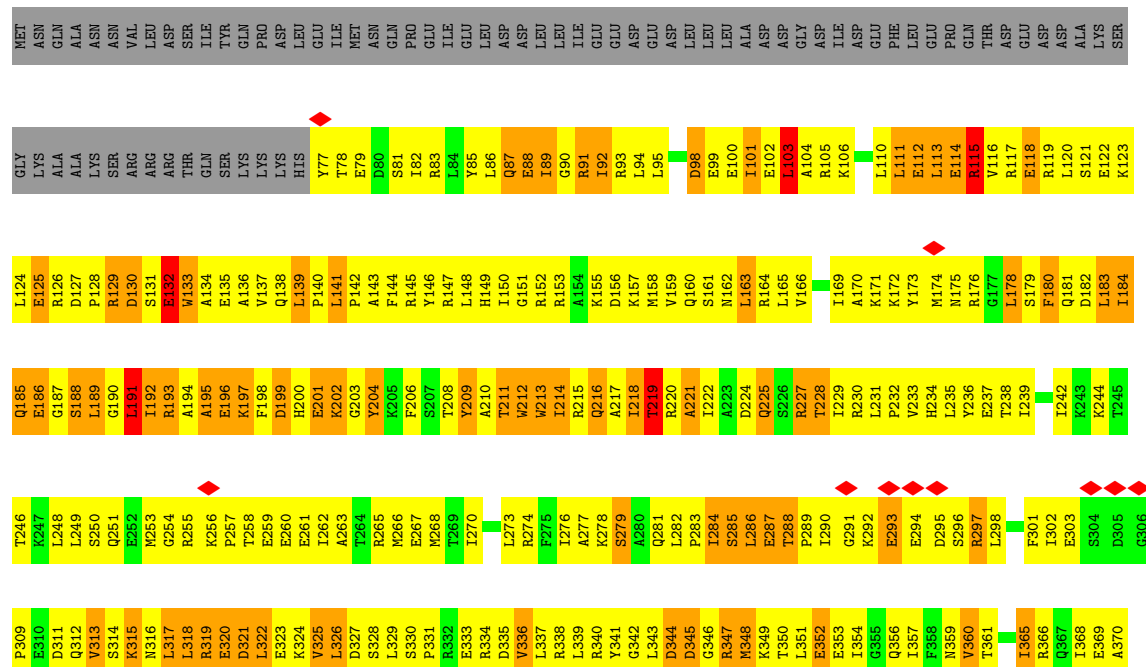


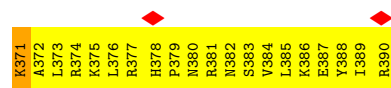


• Molecule 7: DNA-directed RNA polymerase subunit omega

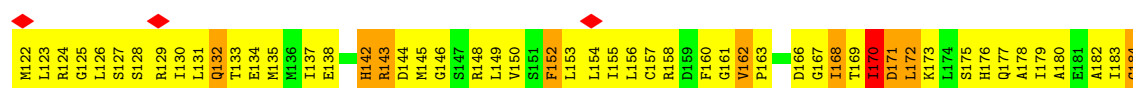
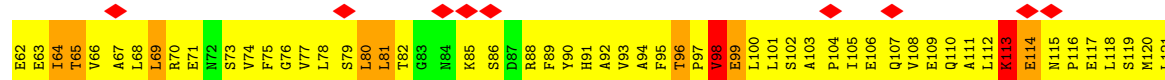
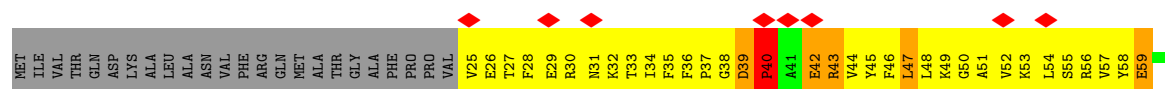
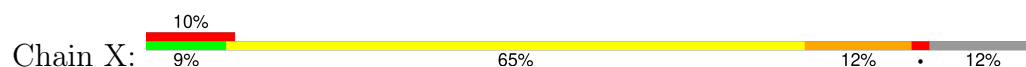


• Molecule 8: RNA polymerase sigma factor SigA

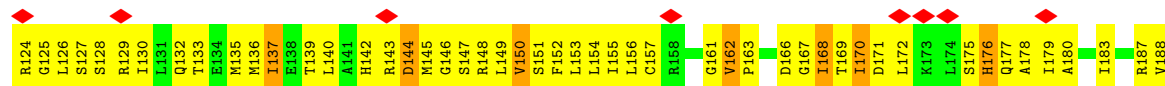
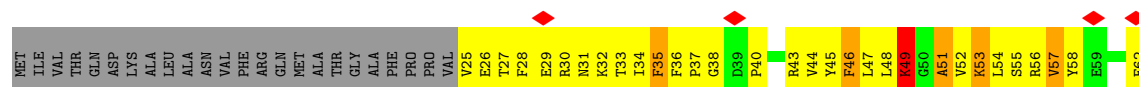
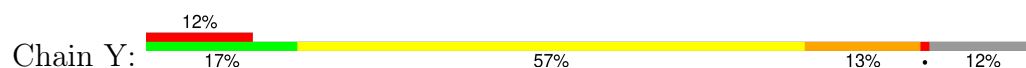




• Molecule 9: NtcA



• Molecule 9: NtcA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45239	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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	1	6.62	598/1523 (39.3%)	2.59	159/2350 (6.8%)
2	2	6.00	432/1244 (34.7%)	2.54	114/1915 (6.0%)
3	A	3.14	815/8632 (9.4%)	1.90	342/11688 (2.9%)
4	B	2.10	345/9414 (3.7%)	1.57	200/12760 (1.6%)
5	C	2.79	124/1788 (6.9%)	1.89	69/2420 (2.9%)
5	D	2.95	144/1788 (8.1%)	1.95	73/2420 (3.0%)
6	E	3.21	485/5014 (9.7%)	1.80	189/6789 (2.8%)
7	F	2.32	22/478 (4.6%)	1.46	12/639 (1.9%)
8	G	1.87	81/2635 (3.1%)	1.39	45/3533 (1.3%)
9	X	0.99	8/1563 (0.5%)	1.27	15/2107 (0.7%)
9	Y	0.94	6/1563 (0.4%)	1.27	20/2107 (0.9%)
All	All	3.06	3060/35642 (8.6%)	1.79	1238/48728 (2.5%)

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
1	1	0	1
2	2	0	1
3	A	0	48
4	B	0	87
5	C	0	10
5	D	0	13
6	E	0	17
7	F	0	1
8	G	0	6
9	X	0	5
9	Y	0	6
All	All	0	195

The worst 5 of 3060 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	62	DT	C1'-N1	-26.91	1.09	1.47
2	2	33	DA	N9-C4	-25.87	1.22	1.37
1	1	77	DA	N9-C4	-25.79	1.22	1.37
2	2	66	DA	N9-C4	-25.75	1.22	1.37
2	2	67	DA	O3'-P	24.28	1.90	1.61

The worst 5 of 1238 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Y	120	MET	CA-CB-CG	-20.38	78.66	113.30
9	X	113	LYS	CD-CE-NZ	-20.09	65.49	111.70
4	B	1018	LEU	CA-CB-CG	-19.77	69.82	115.30
4	B	239	LEU	CA-CB-CG	-19.46	70.55	115.30
9	X	172	LEU	CB-CG-CD1	18.29	142.09	111.00

There are no chirality outliers.

5 of 195 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	100	DA	Sidechain
2	2	67	DA	Sidechain
3	A	51	ASN	Peptide
3	A	52	SER	Mainchain
3	A	75	LYS	Peptide

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	1	1358	0	694	737	0
2	2	1109	0	574	622	0
3	A	8473	0	8480	2770	0
4	B	9292	0	9457	3586	0
5	C	1762	0	1772	621	0
5	D	1762	0	1772	616	0
6	E	4923	0	4987	1470	0
7	F	474	0	477	96	0
8	G	2600	0	2685	873	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	X	1540	0	1613	549	0
9	Y	1540	0	1616	480	0
All	All	34833	0	34127	11682	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 170.

The worst 5 of 11682 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)
4:B:125:MET:HG2	6:E:515:LEU:CD2	1.24	1.65
9:X:42:GLU:CB	9:X:78:LEU:HB3	1.25	1.64
9:Y:78:LEU:CD2	9:Y:88:ARG:HG2	1.15	1.62
3:A:74:LEU:HD21	3:A:95:MET:CG	1.14	1.60
6:E:28:ARG:NH2	6:E:102:ARG:CD	1.67	1.57

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	
3	A	1075/1132 (95%)	634 (59%)	407 (38%)	34 (3%)	3	25
4	B	1209/1350 (90%)	684 (57%)	466 (38%)	59 (5%)	2	17
5	C	224/236 (95%)	131 (58%)	84 (38%)	9 (4%)	2	21
5	D	224/236 (95%)	144 (64%)	72 (32%)	8 (4%)	3	23
6	E	618/625 (99%)	405 (66%)	195 (32%)	18 (3%)	3	27
7	F	56/78 (72%)	36 (64%)	19 (34%)	1 (2%)	7	35
8	G	312/390 (80%)	201 (64%)	100 (32%)	11 (4%)	3	24
9	X	194/223 (87%)	122 (63%)	61 (31%)	11 (6%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Y	194/223 (87%)	124 (64%)	64 (33%)	6 (3%)	3	26
All	All	4106/4493 (91%)	2481 (60%)	1468 (36%)	157 (4%)	4	22

5 of 157 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	615	PRO
3	A	616	THR
3	A	636	ARG
3	A	778	GLU
3	A	890	PRO

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	
3	A	918/969 (95%)	889 (97%)	29 (3%)	34	61
4	B	1017/1132 (90%)	983 (97%)	34 (3%)	33	61
5	C	196/205 (96%)	189 (96%)	7 (4%)	30	59
5	D	196/205 (96%)	189 (96%)	7 (4%)	30	59
6	E	534/538 (99%)	510 (96%)	24 (4%)	23	53
7	F	50/69 (72%)	50 (100%)	0	100	100
8	G	282/351 (80%)	272 (96%)	10 (4%)	31	60
9	X	172/194 (89%)	167 (97%)	5 (3%)	37	63
9	Y	172/194 (89%)	167 (97%)	5 (3%)	37	63
All	All	3537/3857 (92%)	3416 (97%)	121 (3%)	34	60

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	1189	GLN
8	G	387	GLU

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Mol	Chain	Res	Type
5	D	95	GLN
8	G	371	LYS
9	Y	137	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
5	C	93	GLN
5	D	125	GLN
8	G	378	HIS
5	C	125	GLN
5	D	18	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	A	18
6	E	16
4	B	7
5	C	5
5	D	5
8	G	2
2	2	1

The worst 5 of 54 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	67:DA	O3'	68:DT	P	1.90
1	A	144:SER	C	145:PRO	N	1.20
1	E	256:LEU	C	257:ARG	N	1.20
1	E	374:GLY	C	375:LEU	N	1.20
1	A	247:PRO	C	248:PRO	N	1.19

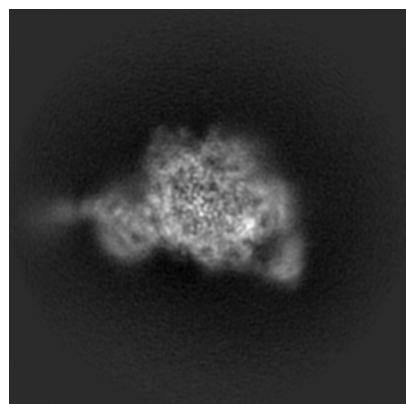
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34476. These allow visual inspection of the internal detail of the map and identification of artifacts.

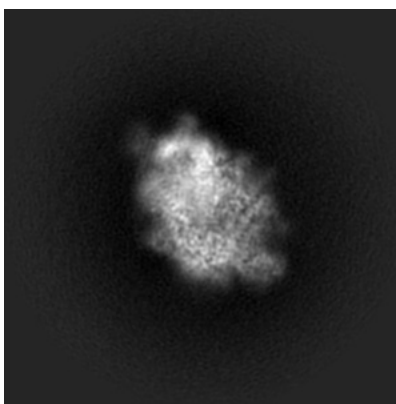
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

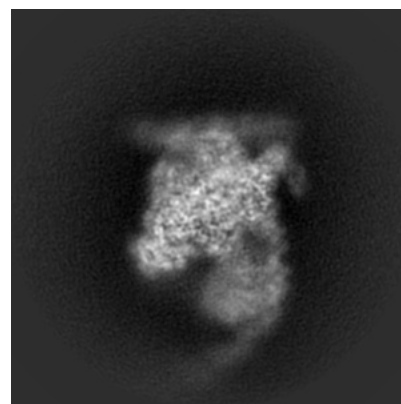
6.1.1 Primary map



X

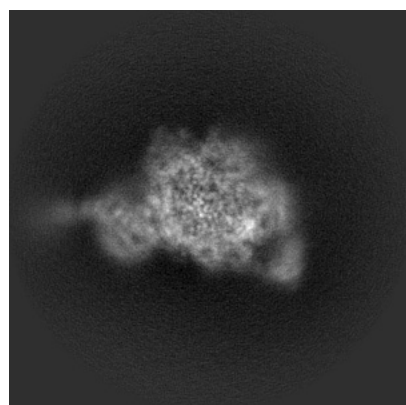


Y

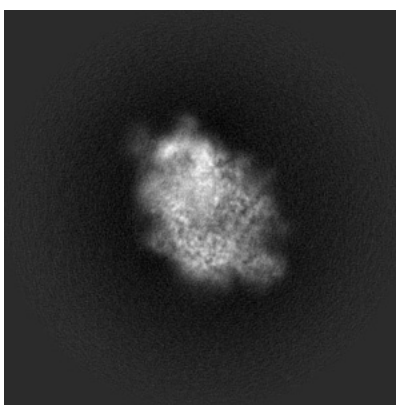


Z

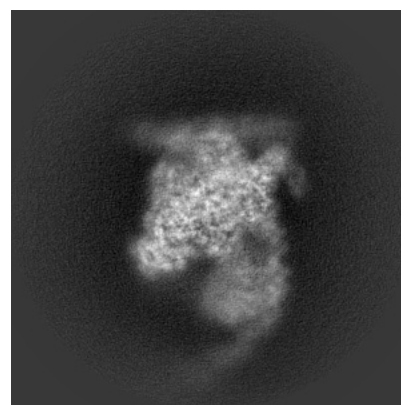
6.1.2 Raw map



X



Y

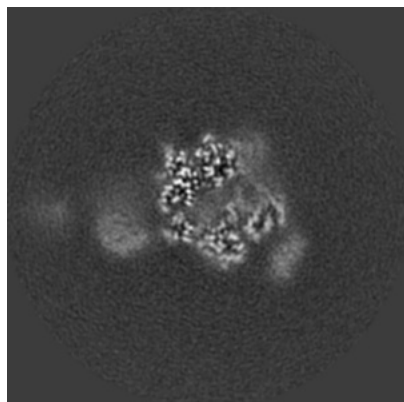


Z

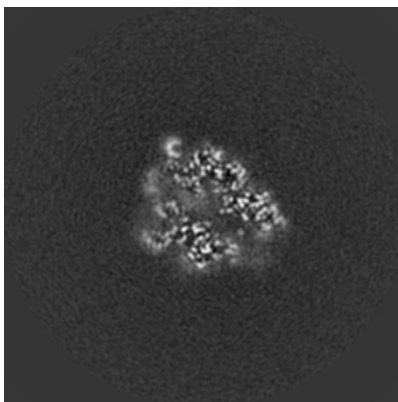
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

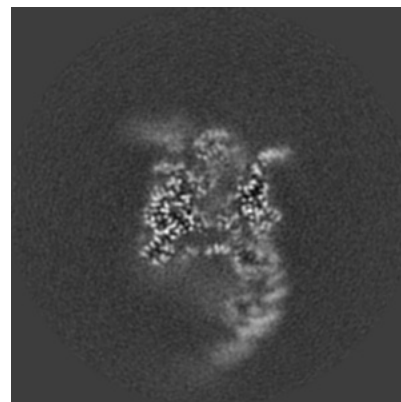
6.2.1 Primary map



X Index: 150

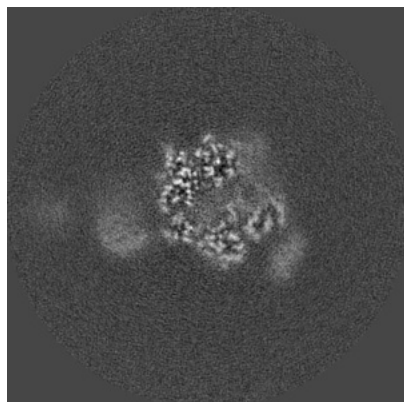


Y Index: 150

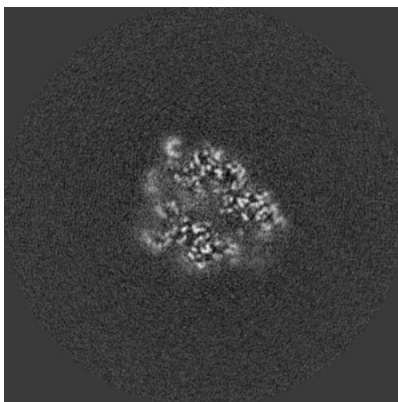


Z Index: 150

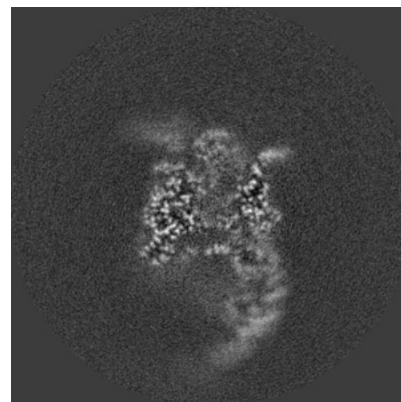
6.2.2 Raw map



X Index: 150



Y Index: 150

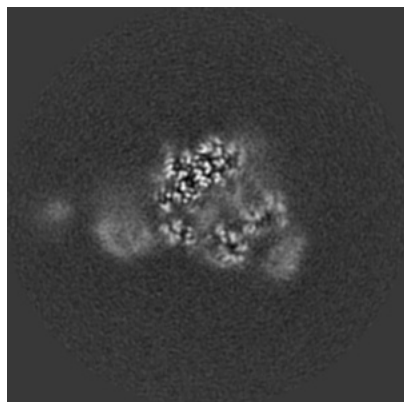


Z Index: 150

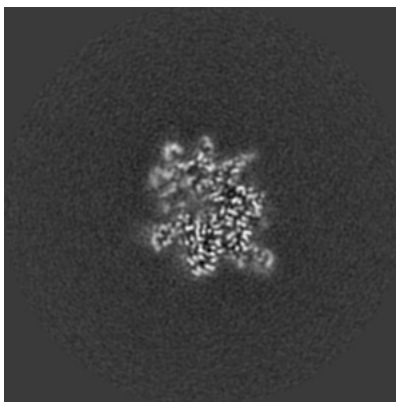
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

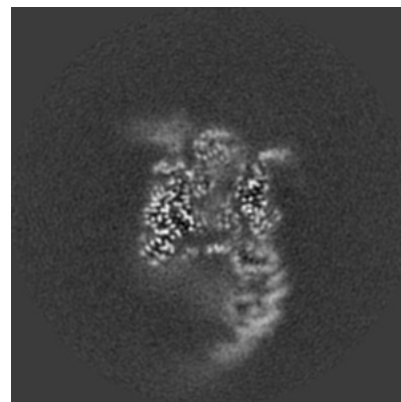
6.3.1 Primary map



X Index: 154

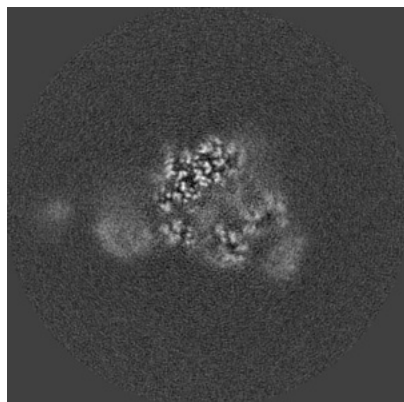


Y Index: 143

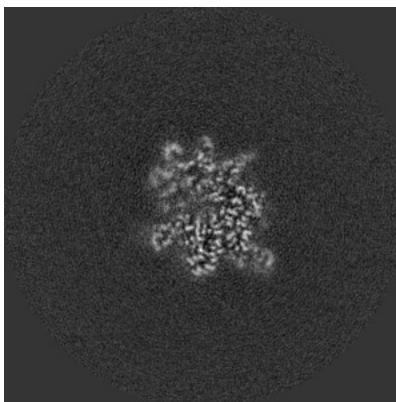


Z Index: 149

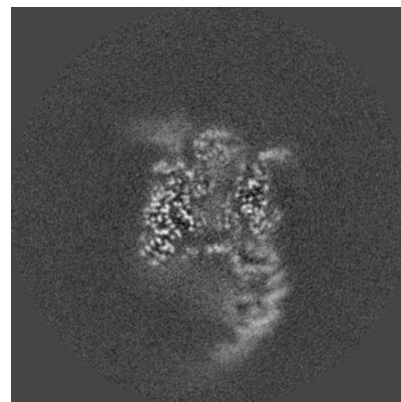
6.3.2 Raw map



X Index: 154



Y Index: 143

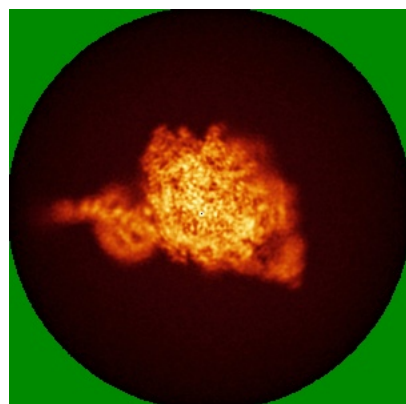


Z Index: 149

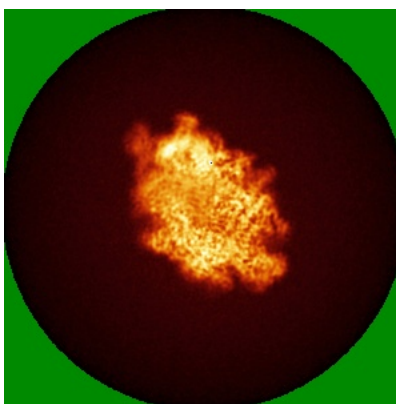
The images above show the largest variance slices of the map in three orthogonal directions.

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

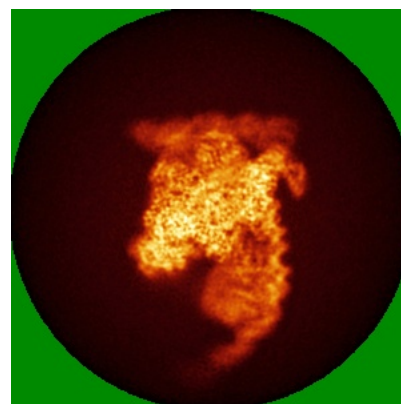
6.4.1 Primary map



X

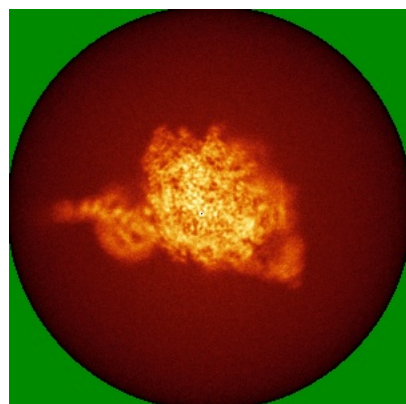


Y

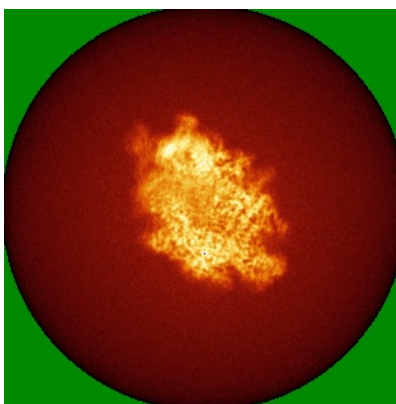


Z

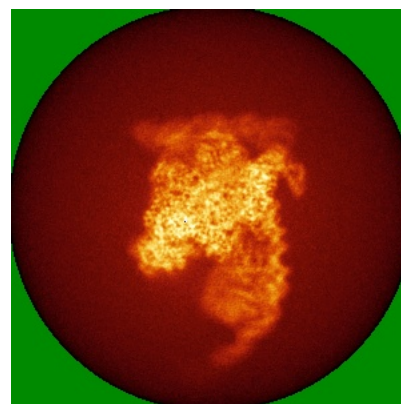
6.4.2 Raw map



X



Y

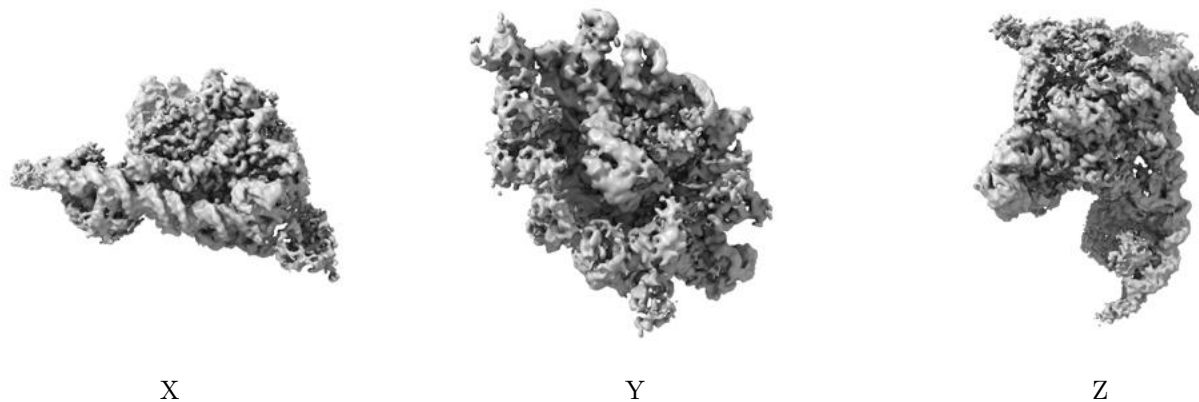


Z

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.

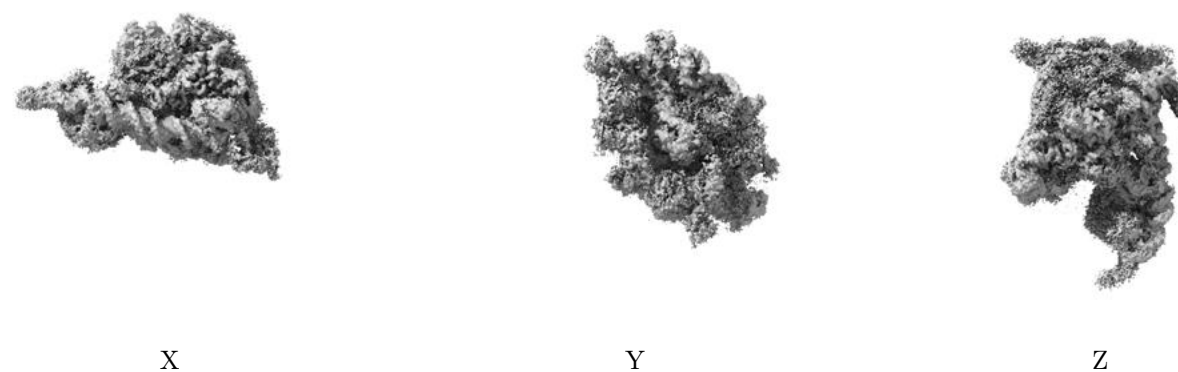
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

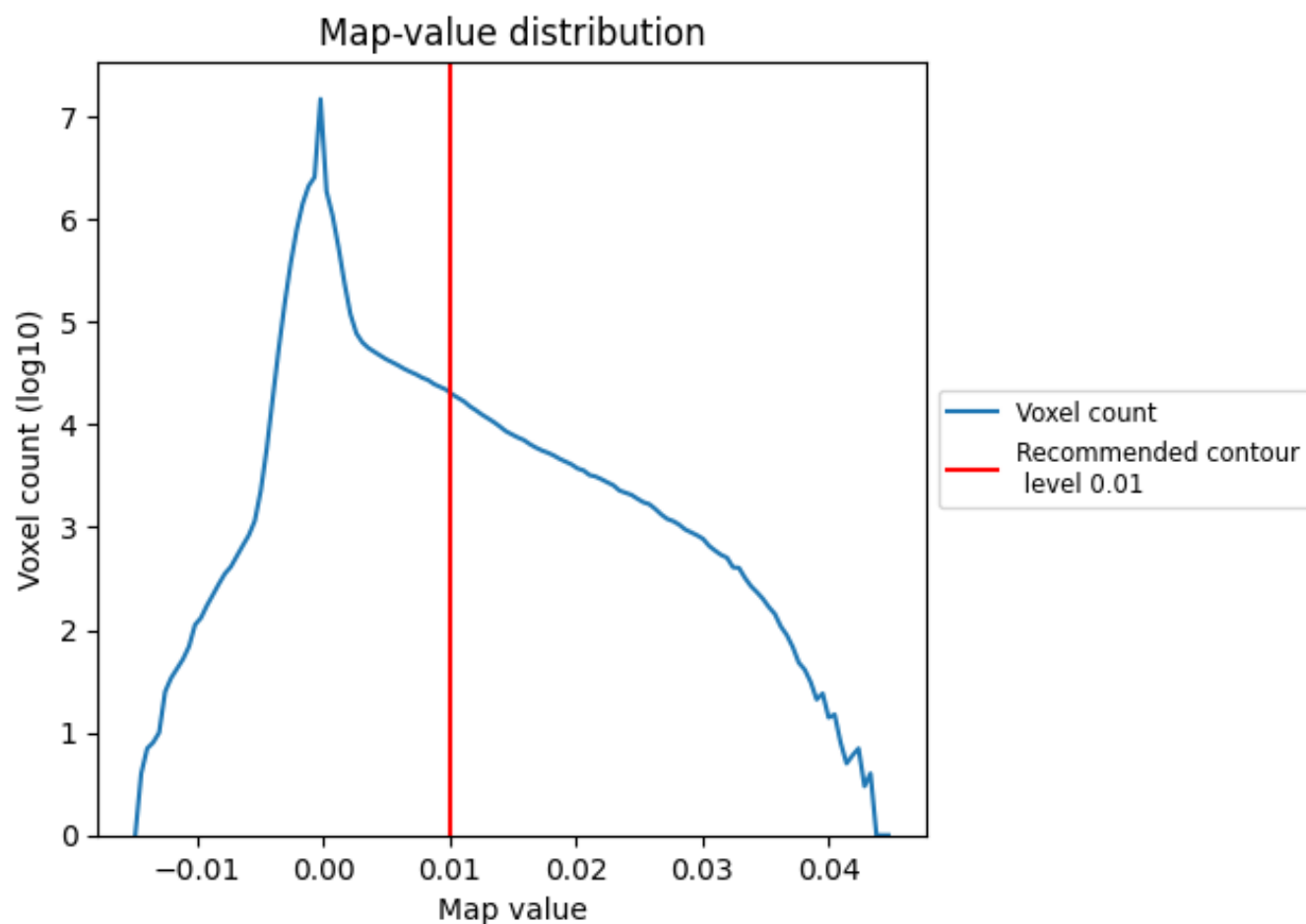
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

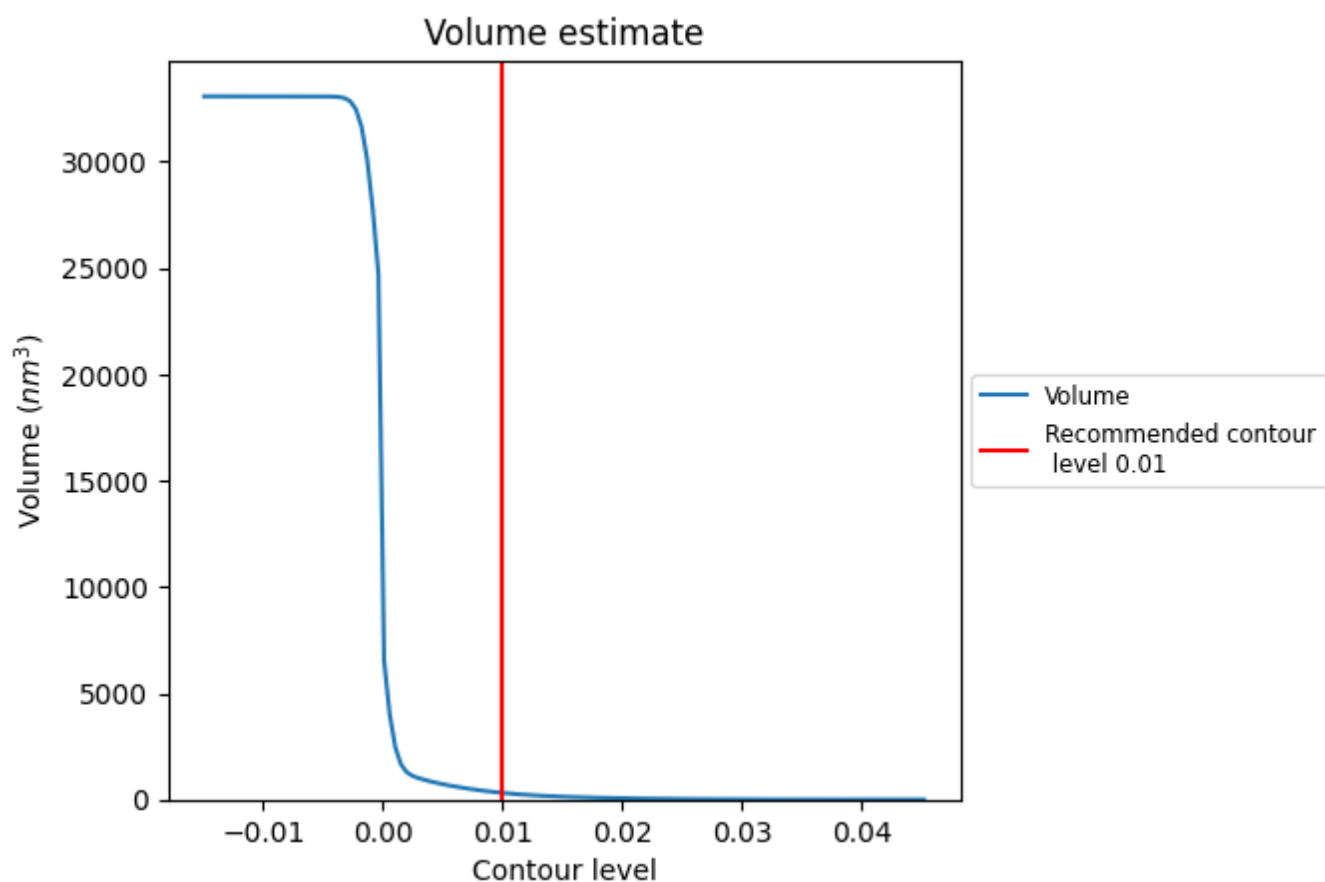
This section contains the results of statistical analysis of the map.

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.

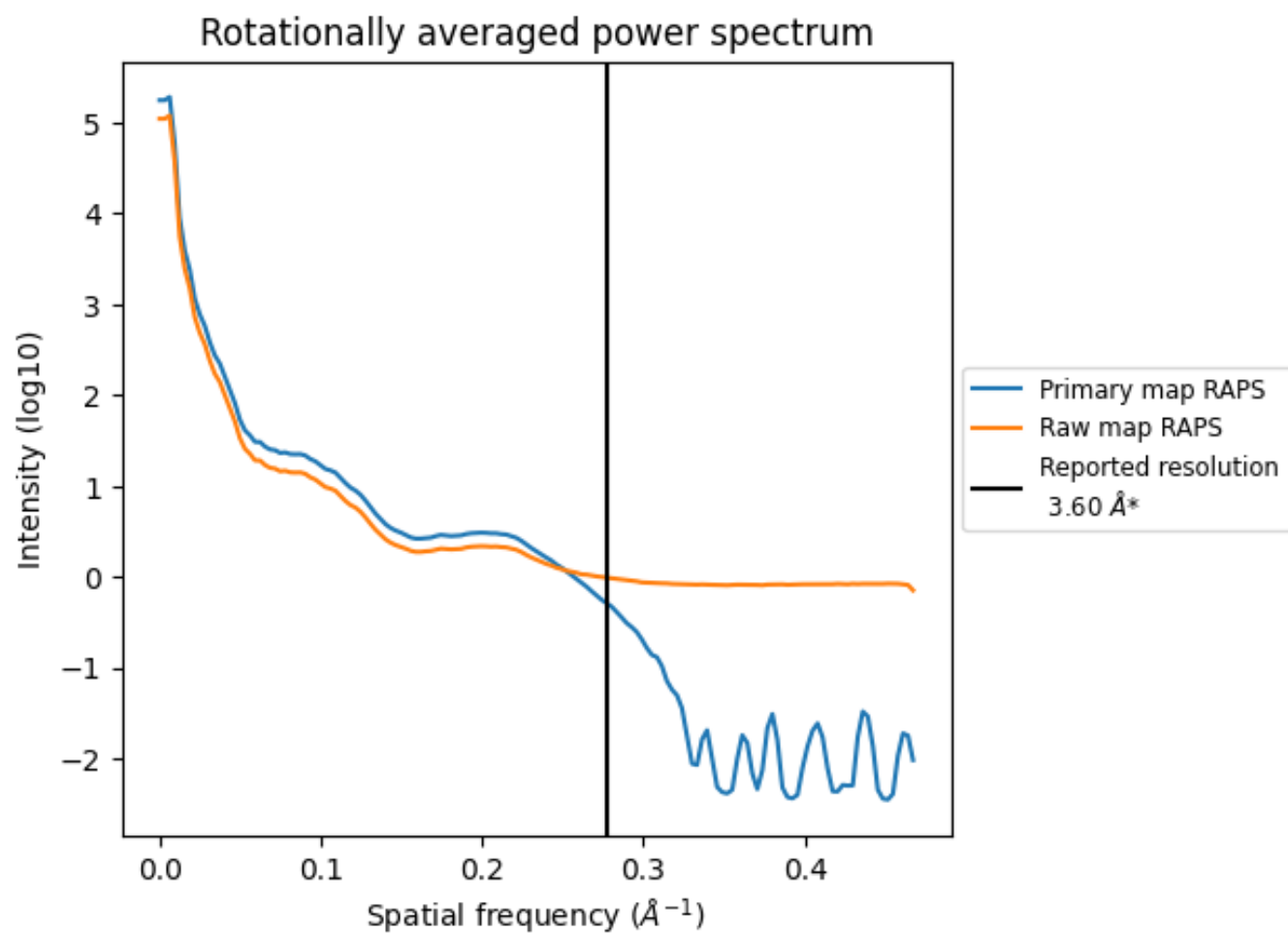
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm³; this corresponds to an approximate mass of 284 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 ⓘ

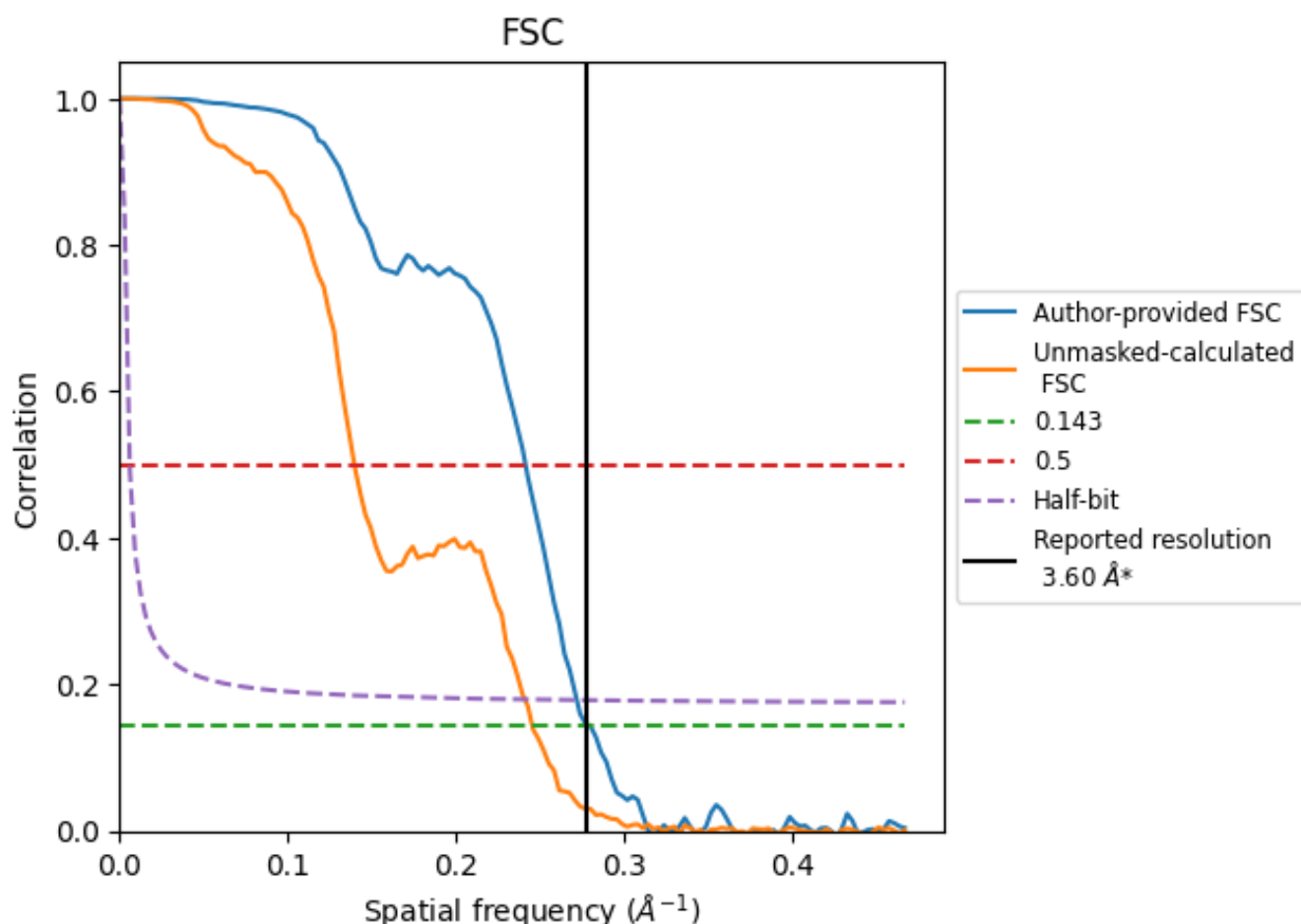


*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

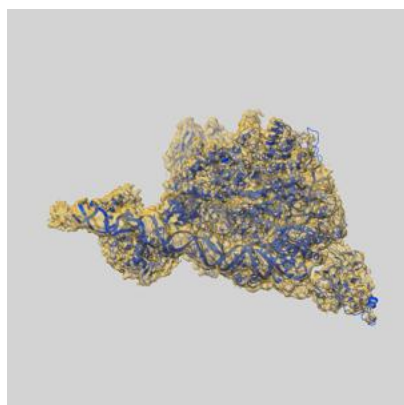
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.14	3.67
Unmasked-calculated*	4.07	7.15	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.6 by more than 10 %

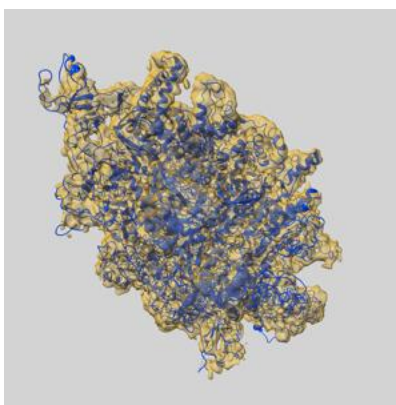
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34476 and PDB model 8H40. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

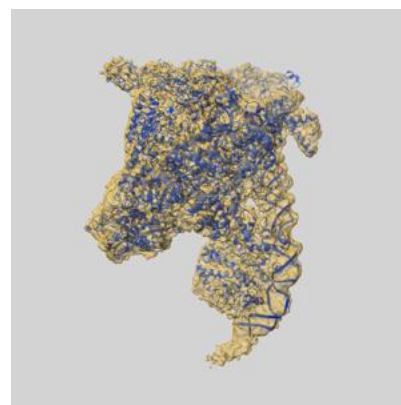
9.1 Map-model overlay [i](#)



X



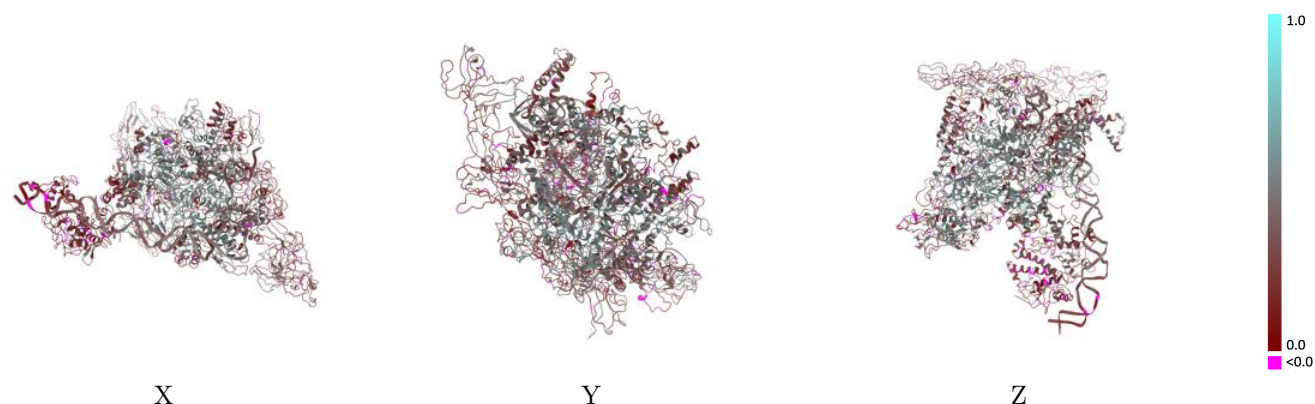
Y



Z

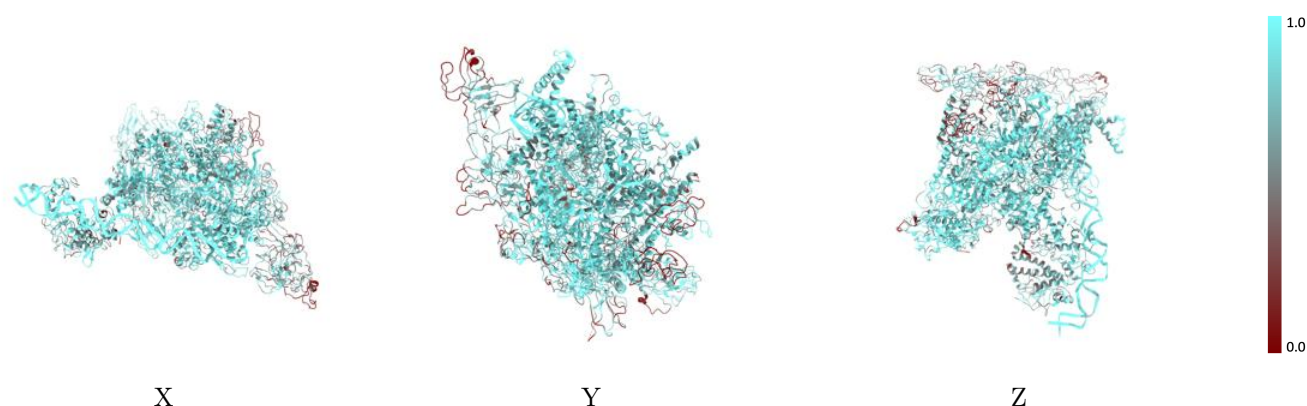
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



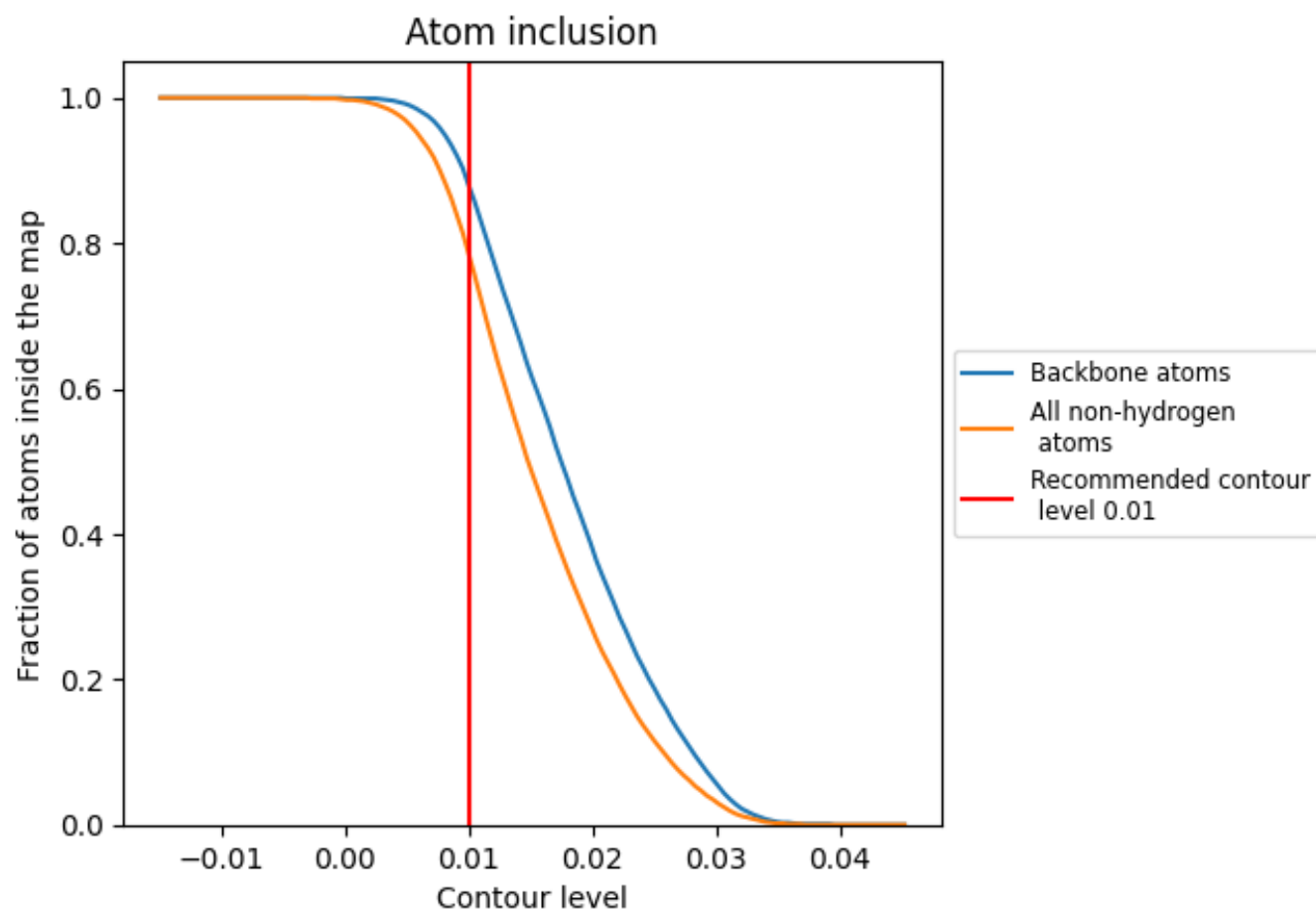
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.3530
1	 0.9600	 0.3610
2	 0.9420	 0.3380
A	 0.8800	 0.4270
B	 0.6250	 0.3320
C	 0.8400	 0.3720
D	 0.8060	 0.3160
E	 0.8600	 0.4120
F	 0.7460	 0.3130
G	 0.8080	 0.3080
X	 0.7120	 0.2080
Y	 0.6830	 0.1450

