



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 06:32 AM UTC

PDB ID : 8H40 / pdb_00008h40
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.

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:

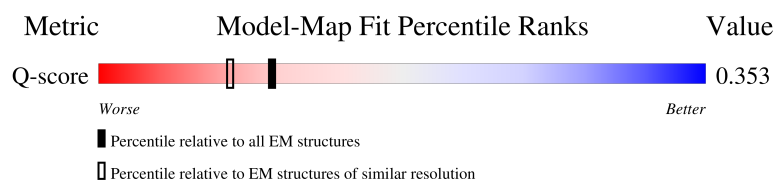
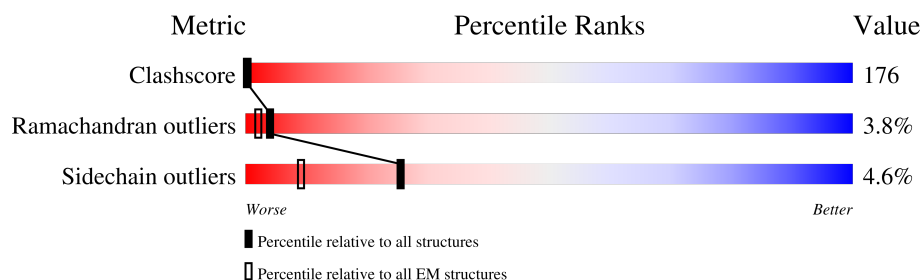
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	
2	2	125	
3	A	1132	
4	B	1350	

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Mol	Chain	Length	Quality of chain
5	C	236	5% 6% 47% 40%
5	D	236	9% 43% 44%
6	E	625	9% 43% 44%
7	F	78	6% 15% 35% 23%
8	G	390	9% 48% 22%
9	X	223	10% 6% 63% 16%
9	Y	223	12% 16% 57% 15%

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		

A1030	D969	H908	V848	L788	A726	G666	I806	EE46	D486	H426	V365	D302	L242	D181
A1031	R970	T909	G549	R789	R727	Q667	R607	H547	D487	Y427	N366	Y303	R243	L182
Y1032	P971	L910	K850	A790	Q728	L668	R608	D548	R488	G428	P367	L304	P244	W183
T1033	P972	G911	D551	A791	T729	L669	R609	D549	R489	R429	K368	I305	G245	W184
L1034	T973	V912	M852	T792	K730	A670	V610	D550	A490	C430	P369	N306	E246	V185
Q1035	T974	R913	A853	G793	L731	D671	S611	N551	A491	C431	L370	L307	P247	R186
E1036	G975	F914	G854	E794	G732	G672	S612	R552	P492	P432	V371	E308	P248	L187
L1037	V976	K915	L733	K795	P733	S673	G613	A553	G493	I433	A372	Y309	T249	D188
L1038	A977	R916	H856	A796	E734	S674	Q613	E434	D494	I434	G379	D310	V250	K189
L1039	G978	T917	G857	R797	E735	T675	L614	M555	I495	T435	I374	I311	L251	T190
V1040	M979	R918	N858	D798	I736	E676	P615	G556	P496	P436	K375	G312	G252	R191
K1041	F919	V919	G859	V799	T737	G677	P616	S557	V497	E437	E376	S313	G253	K192
S1042	R800	R800	G860	R800	R738	G678	A617	N558	D498	G438	F377	I314	Q254	K193
D1043	E921	E921	I861	D801	E739	E679	S618	M559	E499	P439	F378		Q255	S194
D1044	R922	R922	I862	N802	I740	L680	G619	Q660	M501	N440	G379	H319	L256	
M1045	G923	S803	S863	S803	P741	A681	K620	R561	G501	A441	S380	L320	L257	A195
Q1046	L985	L904	R864	L804	N742	G682	S621	E562	I502	G442	L257	G321	D258	Q196
G1047	V986	R805	I865	R805	V743	Q683	T622	A563	I503	L443	S381	R322	S259	V197
R1048	D687	V806	G744	V806	E745	Q684	D623	I504	I444	I444	L383	R323	R260	L198
N1049	E926	P807	E746	P807	D746	L666	D624	G505	G445	G445	S384	R324	F261	
E1050	R988	N808	D746	N808	A747	V687	N624	P506	S446	S446	Q385	R325	F262	K200
A1051	E989	G809	A747	G809	L748	K568	Q626	V508	A447	A447	M387	R326	P263	
L1052	H991	E810	L748	E810	R749	P569	Q625	P509	T449	T449	Q388	S327	P264	L201
N1053	A992	K811	G812	K811	L749	E690	L627	V510	H450	H450	Q389	V328	K265	L202
A1054	R993	V932	R813	V932	Q750	M891	T628	R511	A451	A451	T380	G329	R266	G203
I1055	S994	H933	V814	H933	L751	P692	S629	P572	R452	R452	P391	E330	Y267	L204
V1056	T995	G934	V815	T995	D752	M930	Q630	L573	V453	V453	L331	L332	D268	S205
K1057	G996	K935	P875	K935		E694	K631	V574	N454	N454	L393	Q333	D269	D206
P1058	P997	D876	D876	D876		G695	X631	E575	A394	A394	L394	Q334	G270	N207
K1059	G998	R877	R877	R877		V696	Q633	T576	E456	E456	L395	Q335	V272	E208
A1060	S999	S878	S878	S878		R758	E634	G577	G457	G457	L397	V336	G273	L209
I1061	L1000	E938	R879	L818		E698	E635	L578	F458	F458	H398	R337	R274	F210
V1062	V1001	R940	V880	F820		E579	R636	T519	L459	L459	G339	V338	Y275	D211
G1065	T1002	R882	D881	R821		G600	R637	T520	P521	P521	R400	G339	K276	R214
T1066	Q1003	E942	L882	R822		A701	T638	Q581	P521	P521	R401	L340	L277	H215
P1067	Q1004	T943	L884	Q824		I702	T639	E522	E522	E522	R402	N341	N278	P216
E1068	L1006	K945	N885	G825		L703	V639	Q523	Q523	Q523	L402	R342	K279	E217
S1069	G1007	D946	L887	E826		I704	S640	R584	V524	R464	S403	L343	K280	Y218
F1070	E1008	R947	R887	E827		E706	K641	D585	D525	P465	L405	E344	R282	F219
K1071	A1009	V948	G888	L828		R707	Y642	S586	Y526	V466	G406	R345	L283	Q220
V1072	A1010	Y949	V889	R829		L708	Q643	M588	A528	N468	G409	I347	S284	K221
L1073	Q1011	N950	P890	P830		V709	R644	V589	V529	G469	L410	R348	V285	T222
M1074	Q1012	P951	S891	G831		Q710	N646	V591	S530	R471	T411	E349	E286	I223
L1075	G1013	D952	R892	A832		D711	Q647	S592	V532	R472	R412	R350	E224	E224
E1076	G1014	D953	N833	N833		L712	D648	R593	Q533	F473	E413	V352	E226	E226
Q1015	Q1015		M834	M834		T713	T849	T594	I534	D474	R414	V353	G227	G227
R1016	R1016		V835	V835		Y114	C650	T594	V535	Q475	A415	V353	R290	R290
S1079	F1017	P957	V895	V836		T715	L651	D595	S536	P477	G416	D355	V291	Q228
L1080	G1018	K956	G896	R837		S716	N652	G596	S536	A477	F417	L292	S230	F229
G1081	E1021	M958	Q897	V838		I717	Q653	D597	V537	A477	A356	L293	S230	Q229
L1082	V1022	Y960	V898	Y839		H718	K654	V598	A538	A478	A418	T293	E231	E231
T1083	G1023	D961	R899	V840		T719	P655	V599	T539	Y479	V419	E357	E232	E232
A1085	A1024	R963	C901	A841		E720	L656	Y600	S540	M480	R420	V358	G295	E233
V1086	L1025	Q942	L902	Q842		K721	V657	V601	M541	T481	D421	L359	D296	A234
H1087	E1026	R844	L903	R844		Y722	R658	D602	I542	I422	I422	T360	L298	L235
K1088	Q1027	G965	G904	K845		E723	I659	A603	P543	A482	H423	P361	A299	M236
V1089	F1028	A967	W905	I846		T724	G660	T604	F544	E484	P424	S363	A300	E237
E1090	G1029	F968	A906	Q847		E725	E861	E605	L545	E485	S425	P424	L238	L238
			G907				V663						R240	K241
							A665							

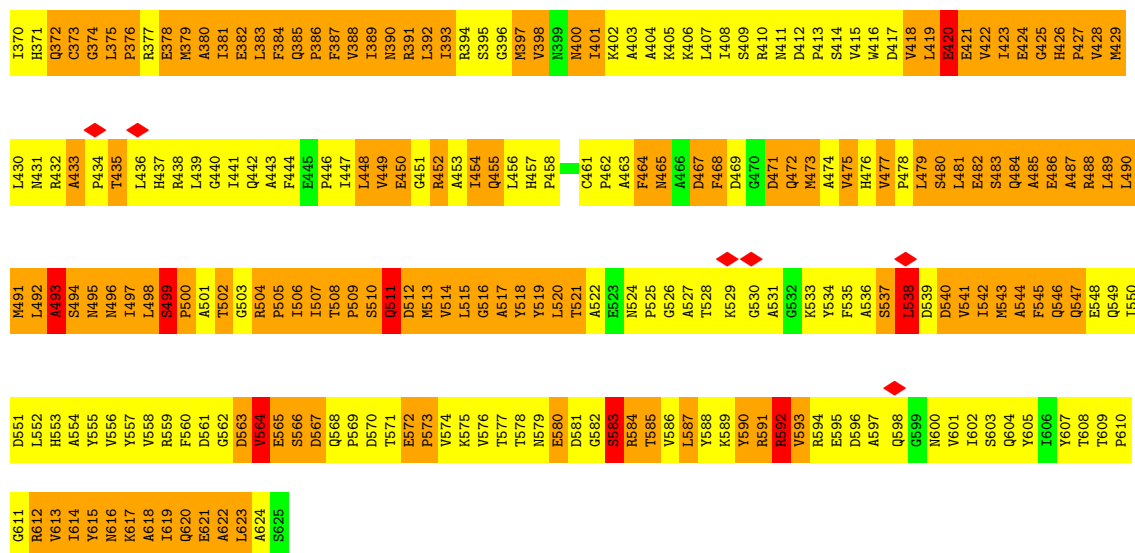
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● Molecule 4: DNA-directed RNA polymerase subunit beta'

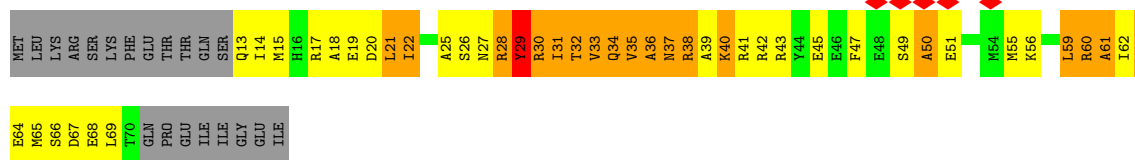


M1	I2	F3	R4	N5	R6	V7	V8	D9	K10	G11	Q12	L13	R14	M15	L16	I17	S18	W19	A20	F21	G22	H23	Y24	G25	T26	A27	R28	T29	A30	M31	A32	D33	K34	L35	K36	L37	D38	L39	G40	F41	R42	Y43	T44	R45	A46	G47	V48	S49	I50	S51	S52	V53	L54	M55	V56	P57	P58	S59	S60			
K62	R63	S64	L65	L66	E67	A68	E69	E70	E71	E72	I73	Q74	A75	T76	E77	R78	V79	Y80	Q81	R82	G83	E84	I85	T86	E87	V88	E89	R90	F91	Q92	K93	V94	I95	D96	T97	N98	N99	G100	T101	S102	E103	A104	L105	K106	D107	E108	V109	V110	T111	H112	I113	F113	K114	M115	P116	L117	V118	N119	P120	P121	V122	
Y123	M124	A125	F126	A127	S128	R129	L130	Q131	G132	E133	N134	K135	L136	V137	R138	Q139	V140	L141	G142	M143	R144	G145	L146	M147	A148	D149	P150	Q151	G152	E153	K154	I155	D156	L157	P158	I159	K160	T161	N162	F163	R164	E165	G166	L167	T168	V169	T170	E171	Y172	I173	T174	S175	S176	Y177	G178	A179	R180	L181	G182	L183		
V184	D185	T186	A187	L188	R189	T190	A191	D192	S193	G194	L195	T196	L197	R198	R199	L200	V201	D202	V203	S204	Q205	D206	V207	T208	A209	K210	E211	Q212	D213	C214	G215	T216	G219	T220	P221	V222	N223	P224	M225	T226	E227	G228	S229	K230	T231	L232	L233	K234	L235	S236	T237	R238	L239	L240	G241	R242	S243	V244				
G245	E246	D247	V248	L249	H250	P251	K252	K253	K254	E255	V256	T257	K258	P259	R260	R261	L262	V263	T264	S265	D266	D267	L268	A269	K270	E271	T272	E273	K274	A275	G276	T277	E278	V280	V281	V282	R283	S284	P285	L286	T287	C288	A289	A290	R291	R292	S293	V294	C295	Q296	H297	C298	V299	G300	W301	K302	L303	A304				
H305	A306	K307	K308	V309	D310	L311	G312	E313	A314	V315	G316	I317	A318	A319	C320	Q321	S322	G323	G324	E325	P326	G327	T328	Q329	L330	T331	M332	ARG	THR	PHE	HIS	THR	GLY	GLY	VAL	PHE	THR	GLY	VAL	ALA	Q347	Q348	Q349	R350	S351	K352	T353	D354	G355	T356	L357	W358	L359	P360	R361	K362	L363	R364				
T365	R366	T367	H368	R369	T370	R371	H372	G373	E374	ARG	THR	THR	A376	L377	F378	V379	E380	S381	N382	G383	I384	N385	L386	L387	K388	P389	R390	K391	E392	G393	S394	E395	T396	P397	A398	P399	Q400	E401	I402	H403	V404	T405	T406	Q406	Q407	S408	T409	I410	T411	L412	V413	D414	C415	Q416	Q417	V418	R419	K420	G421	Q422	L423	L424
A425	E426	V427	A428	L429	GLY	ARG	THR	THR	ARG	THR	THR	N437	T438	E439	K440	A441	V442	K443	D444	V445	A446	S447	D448	L449	A450	G451	E452	V453	K454	F455	A456	E457	V458	V459	P460	E461	Q462	K463	T464	D465	R466	Q467	G468	T470	T471	T472	T473	A474	A475	R476	G477	G478	L479	I480	W481	L482	L483	S484				
G485	E486	V487	Y488	R489	P491	P492	Q493	A494	E495	L496	V497	V498	K499	N500	G501	D502	R503	V504	E505	T506	N507	G508	V509	L510	A511	E512	T513	K514	L515	T516	T517	V518	H519	G520	E521	V522	V523	R524	L525	P526	E527	A528	T529	P530	G531	S532	S533	T534	R535	E536	E537	E538	V539	I540	T541	G601	A542	L483	S484			
V545	L546	D547	Q548	A549	T550	V551	V552	V553	Q554	S555	S556	Q557	G558	R559	N560	M561	E562	L563	L564	T565	V566	G567	N568	L569	Q570	V571	L572	N573	L574	R575	A576	T577	P578	G579	T580	K581	V582	Q583	N584	G585	Q586	V587	A588	E589	E590	L591	I592	D593	R594	A475	R596	T598	V599	V600	G601	A542	L483	S484				
K605	F606	G607	G608	S609	V610	V611	Q612	K613	K614	G615	G616	A617	K618	L619	G620	Y621	E622	V623	V624	Q625	G626	G627	T628	L629	L630	W631	L632	P633	E634	E635	L636	H637	E638	V639	N640	K641	D642	L643	S644	L645	L646	L647	V648	E649	D650	G651	G652	Y653	V654	E655	E656	G657	T658	E659	V660	V661	K662	D663	L664			
R665	C666	N667	N668	S669	G670	V671	V672	E673	V674	T675	Q676	K677	N678	D679	L680	L681	R682	E683	V684	V685	V686	K687	P688	G689	E690	L691	L692	P693	E694	D695	D696	P697	E698	N699	V700	D642	L643	S644	L645	L646	L647	V648	E649	D650	G651	G652	Y653	V654	E655	E656	G657	T658	E659	V660	V661	K662	D663	L664				
R701	G702	R703	T704	N705	T706	L707	L708	Q709	P710	G711	E712	E713	L714	L715	G716	Q717	V718	A719	T720	E721	L722	R723	Y724																																							

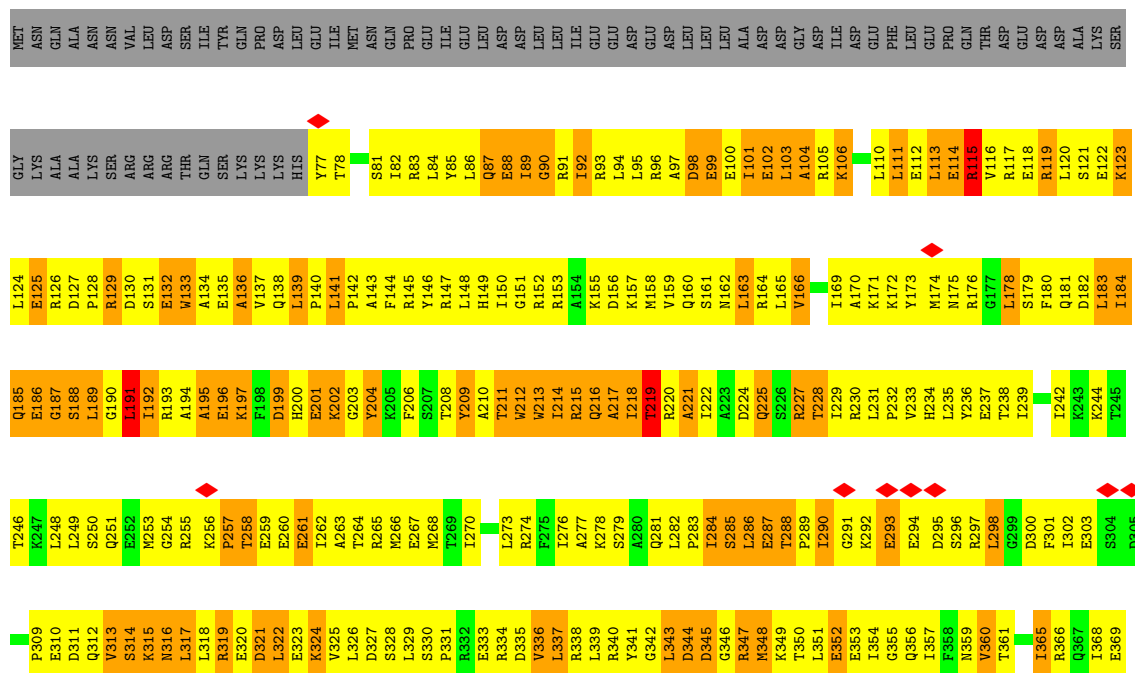




• Molecule 7: DNA-directed RNA polymerase subunit omega



• Molecule 8: RNA polymerase sigma factor SigA





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	2.90	118/1523 (7.7%)	1.53	18/2350 (0.8%)
2	2	2.65	66/1244 (5.3%)	1.53	19/1915 (1.0%)
3	A	3.26	1063/8632 (12.3%)	2.31	597/11688 (5.1%)
4	B	2.17	464/9414 (4.9%)	1.90	362/12760 (2.8%)
5	C	3.03	162/1788 (9.1%)	2.23	99/2420 (4.1%)
5	D	3.14	177/1788 (9.9%)	2.33	112/2420 (4.6%)
6	E	3.35	771/5014 (15.4%)	2.25	311/6789 (4.6%)
7	F	2.50	45/478 (9.4%)	2.02	27/639 (4.2%)
8	G	2.10	108/2635 (4.1%)	1.80	82/3533 (2.3%)
9	X	1.25	4/1563 (0.3%)	1.75	42/2107 (2.0%)
9	Y	1.14	4/1563 (0.3%)	1.66	34/2107 (1.6%)
All	All	2.74	2982/35642 (8.4%)	2.05	1703/48728 (3.5%)

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 2982 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1079	SER	CA-C	-39.16	1.04	1.53
5	D	45	LEU	CA-C	-38.41	0.98	1.52
5	C	45	LEU	CA-C	-38.39	0.98	1.52
6	E	117	TYR	CA-C	-33.36	0.97	1.52
6	E	61	ARG	CA-C	-33.30	1.03	1.52

The worst 5 of 1703 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	80	MET	N-CA-C	-20.41	86.51	112.23
5	D	80	MET	N-CA-C	-20.40	86.53	112.23
6	E	538	LEU	CA-C-N	-19.05	85.16	121.54
6	E	538	LEU	C-N-CA	-19.05	85.16	121.54
9	X	39	ASP	CA-C-N	18.48	142.94	119.84

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	739	0
2	2	1109	0	574	618	0
3	A	8473	0	8481	2897	0
4	B	9292	0	9457	3718	0
5	C	1762	0	1772	647	0
5	D	1762	0	1772	649	0
6	E	4923	0	4987	1511	0
7	F	474	0	477	103	0
8	G	2600	0	2685	909	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	X	1540	0	1613	574	0
9	Y	1540	0	1616	496	0
All	All	34833	0	34128	12119	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 176.

The worst 5 of 12119 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	24
4	B	1209/1350 (90%)	684 (57%)	466 (38%)	59 (5%)	1	16
5	C	224/236 (95%)	131 (58%)	84 (38%)	9 (4%)	2	20
5	D	224/236 (95%)	144 (64%)	72 (32%)	8 (4%)	2	22
6	E	618/625 (99%)	405 (66%)	195 (32%)	18 (3%)	3	26
7	F	56/78 (72%)	36 (64%)	19 (34%)	1 (2%)	6	34
8	G	312/390 (80%)	201 (64%)	100 (32%)	11 (4%)	3	23
9	X	194/223 (87%)	122 (63%)	61 (31%)	11 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Y	194/223 (87%)	124 (64%)	64 (33%)	6 (3%)	3	25
All	All	4106/4493 (91%)	2481 (60%)	1468 (36%)	157 (4%)	4	21

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%)	886 (96%)	32 (4%)	32	57
4	B	1017/1132 (90%)	972 (96%)	45 (4%)	25	52
5	C	196/205 (96%)	188 (96%)	8 (4%)	27	53
5	D	196/205 (96%)	185 (94%)	11 (6%)	19	47
6	E	534/538 (99%)	500 (94%)	34 (6%)	16	43
7	F	50/69 (72%)	49 (98%)	1 (2%)	48	66
8	G	282/351 (80%)	270 (96%)	12 (4%)	26	52
9	X	172/194 (89%)	161 (94%)	11 (6%)	16	43
9	Y	172/194 (89%)	165 (96%)	7 (4%)	27	53
All	All	3537/3857 (92%)	3376 (95%)	161 (5%)	25	51

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	E	177	GLU
9	X	74	VAL

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Mol	Chain	Res	Type
6	E	379	MET
7	F	63	ILE
9	X	194	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
6	E	616	ASN
8	G	175	ASN
9	X	142	HIS
4	B	573	ASN
4	B	560	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

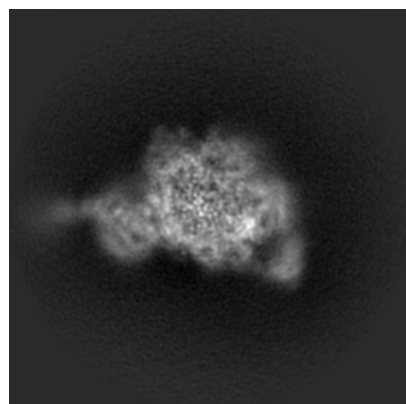
6 Map visualisation [i](#)

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.

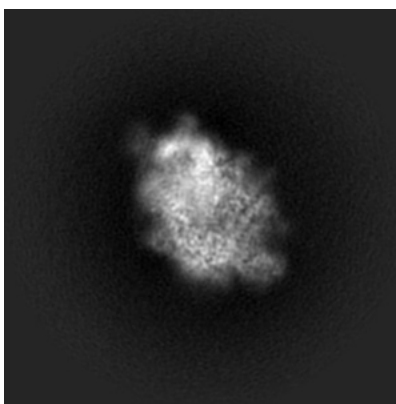
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

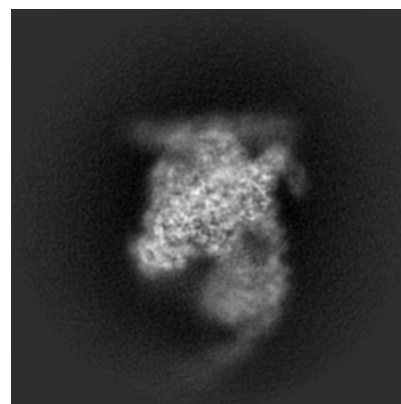
6.1.1 Primary map



X

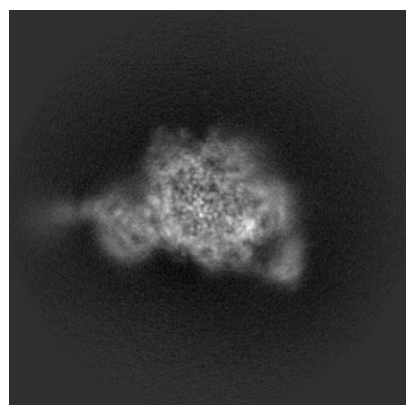


Y

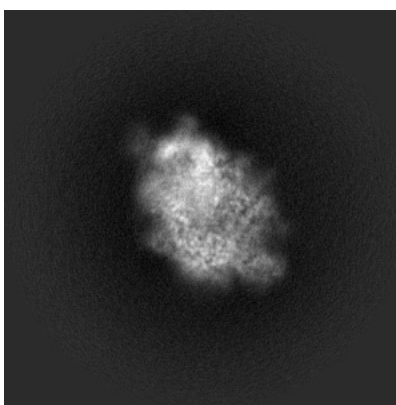


Z

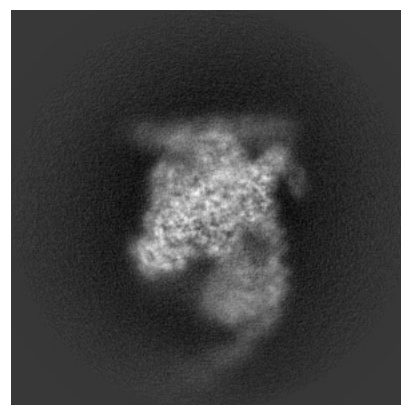
6.1.2 Raw map



X



Y

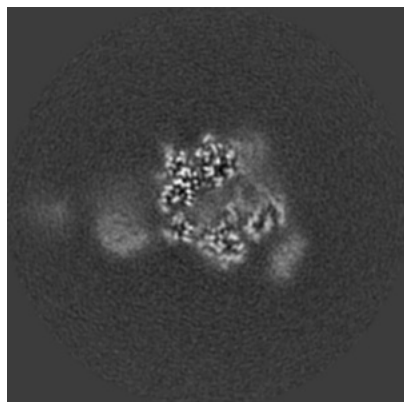


Z

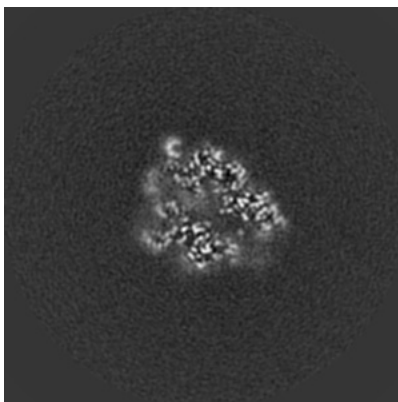
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

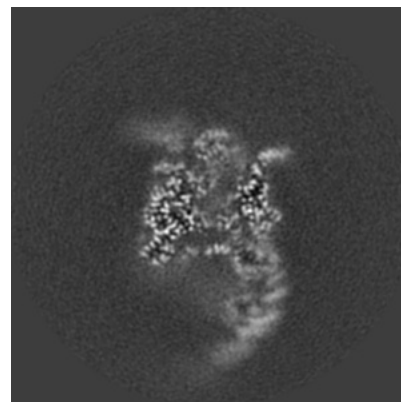
6.2.1 Primary map



X Index: 150

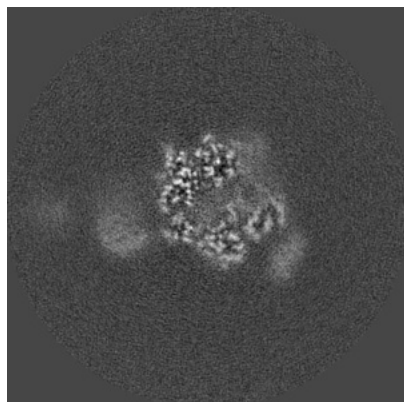


Y Index: 150

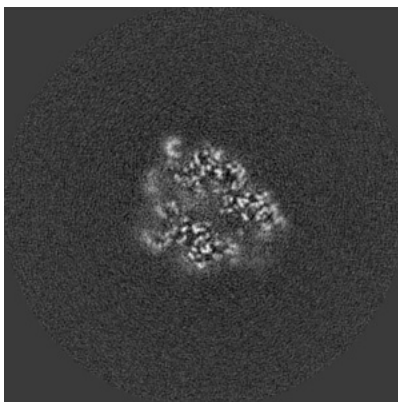


Z Index: 150

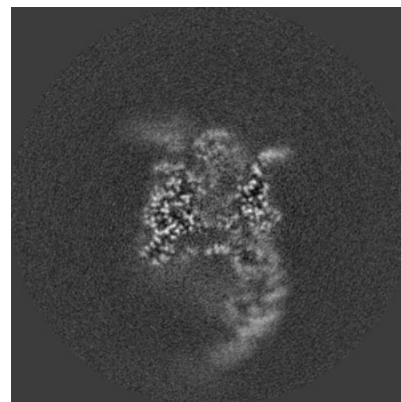
6.2.2 Raw map



X Index: 150



Y Index: 150

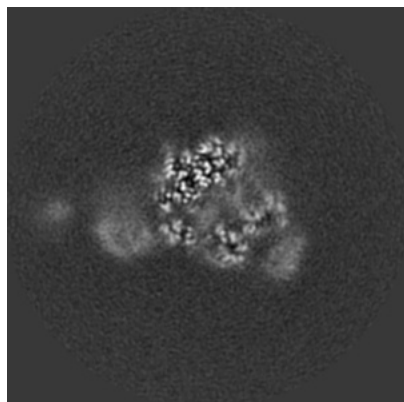


Z Index: 150

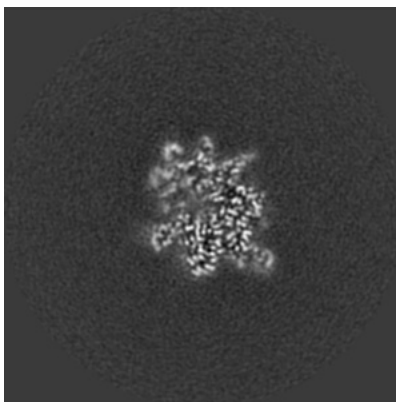
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

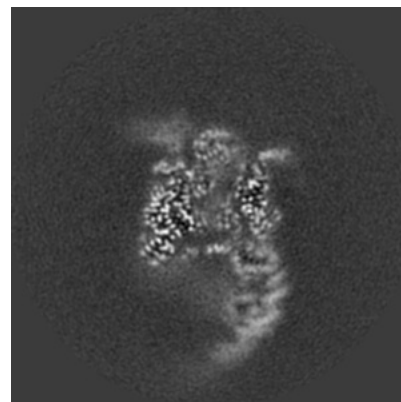
6.3.1 Primary map



X Index: 154

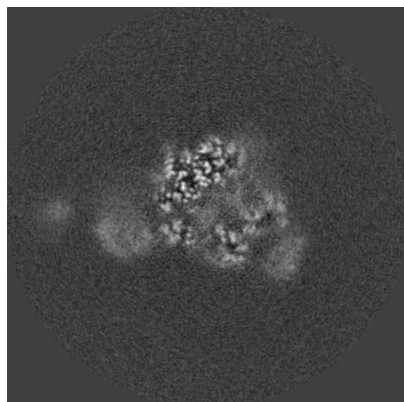


Y Index: 143

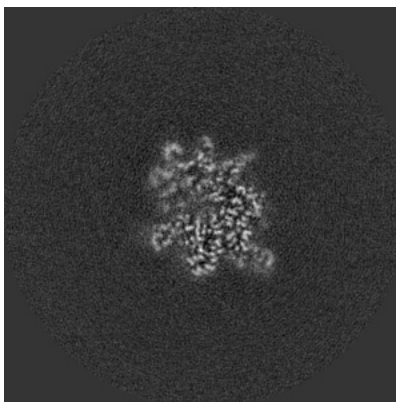


Z Index: 149

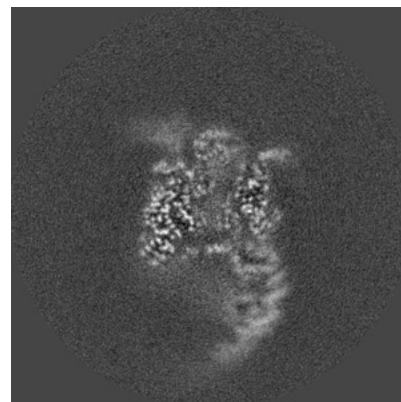
6.3.2 Raw map



X Index: 154



Y Index: 143

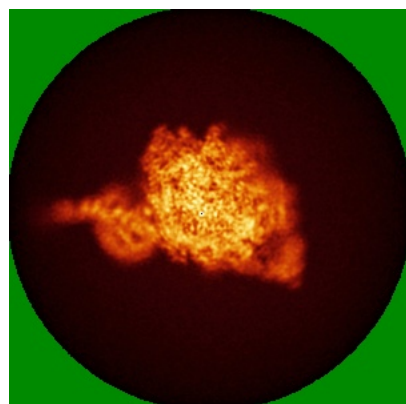


Z Index: 149

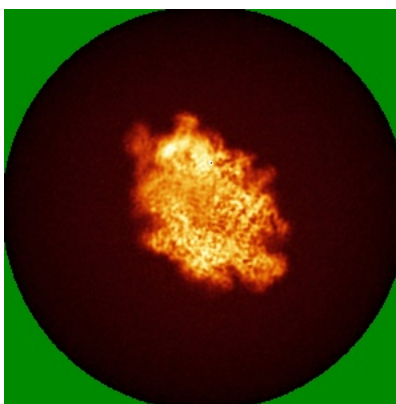
The images above show the largest variance slices of the map in three orthogonal directions.

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

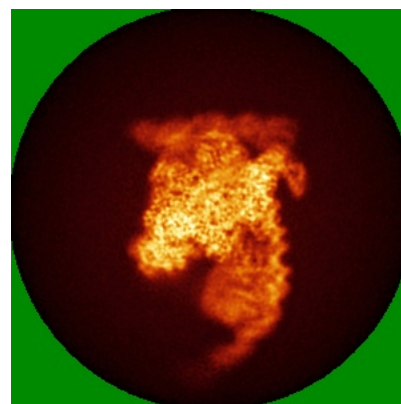
6.4.1 Primary map



X

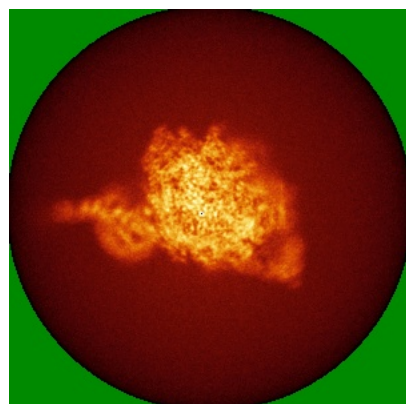


Y

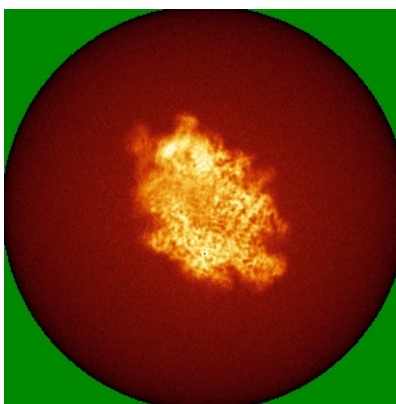


Z

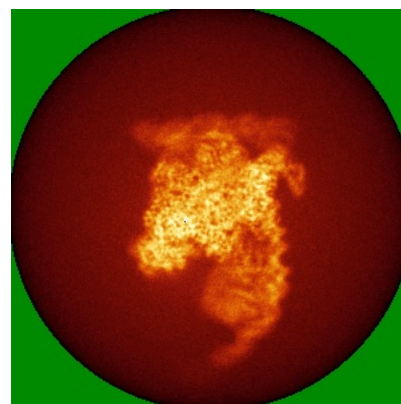
6.4.2 Raw map



X



Y

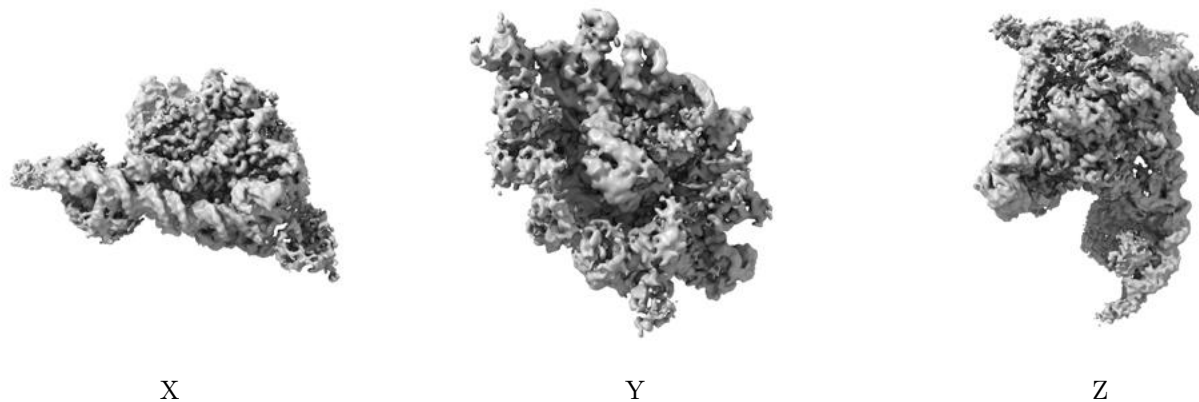


Z

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.

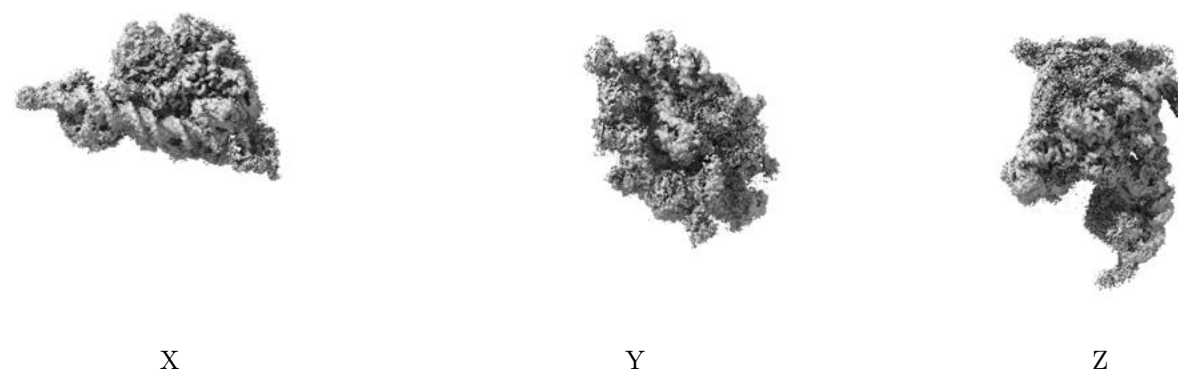
6.5 Orthogonal surface views [i](#)

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.

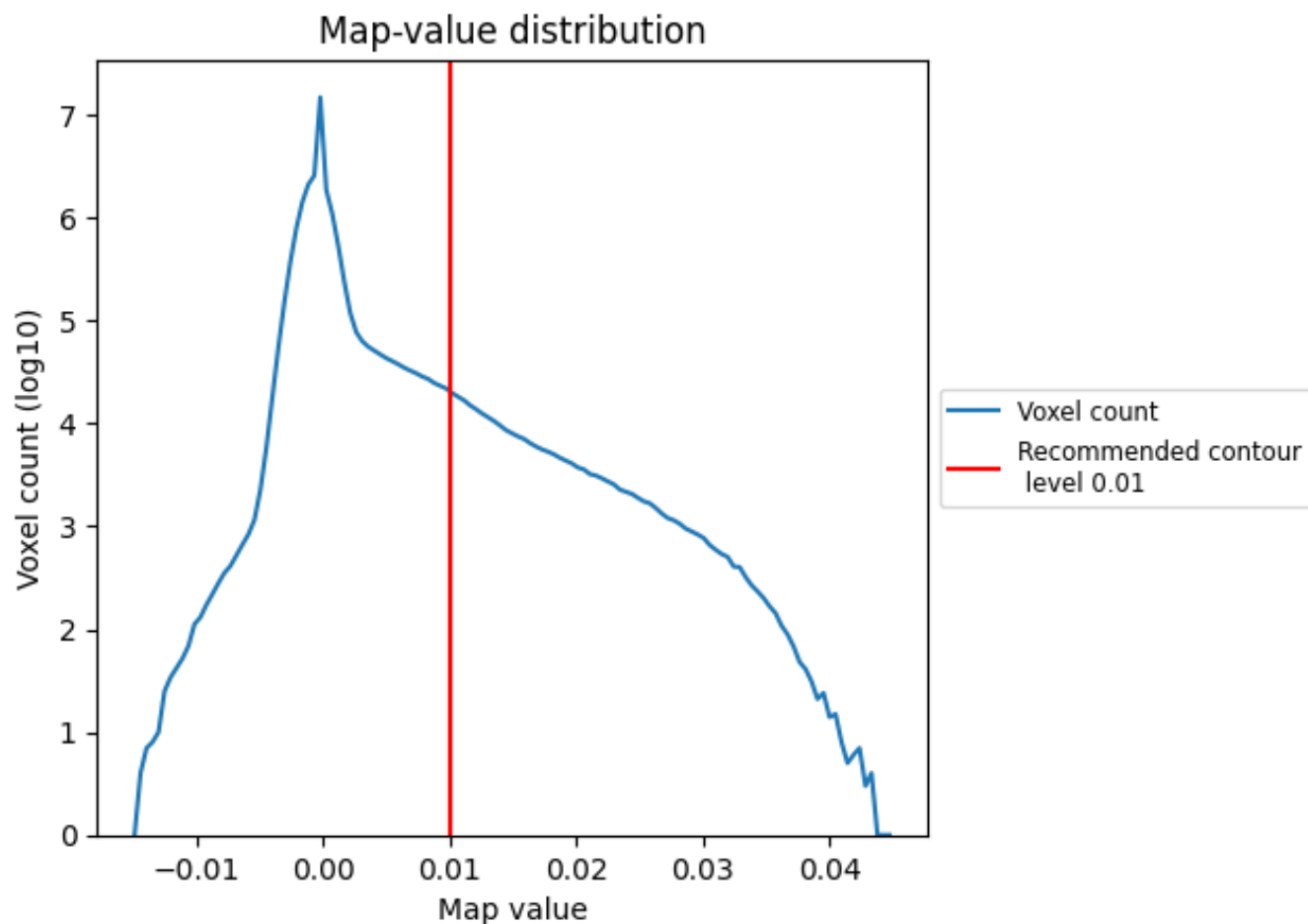
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

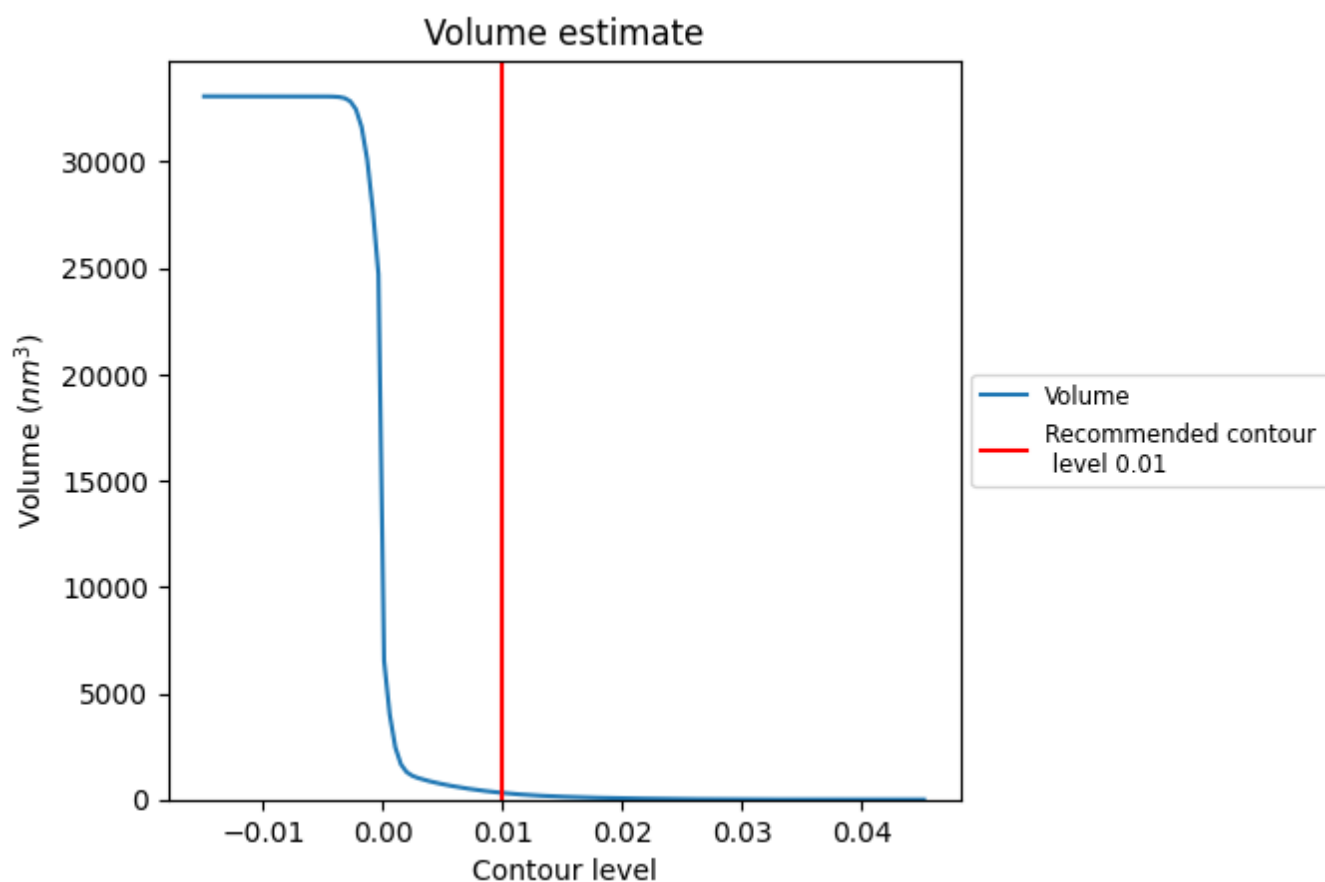
This section contains the results of statistical analysis of the map.

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.

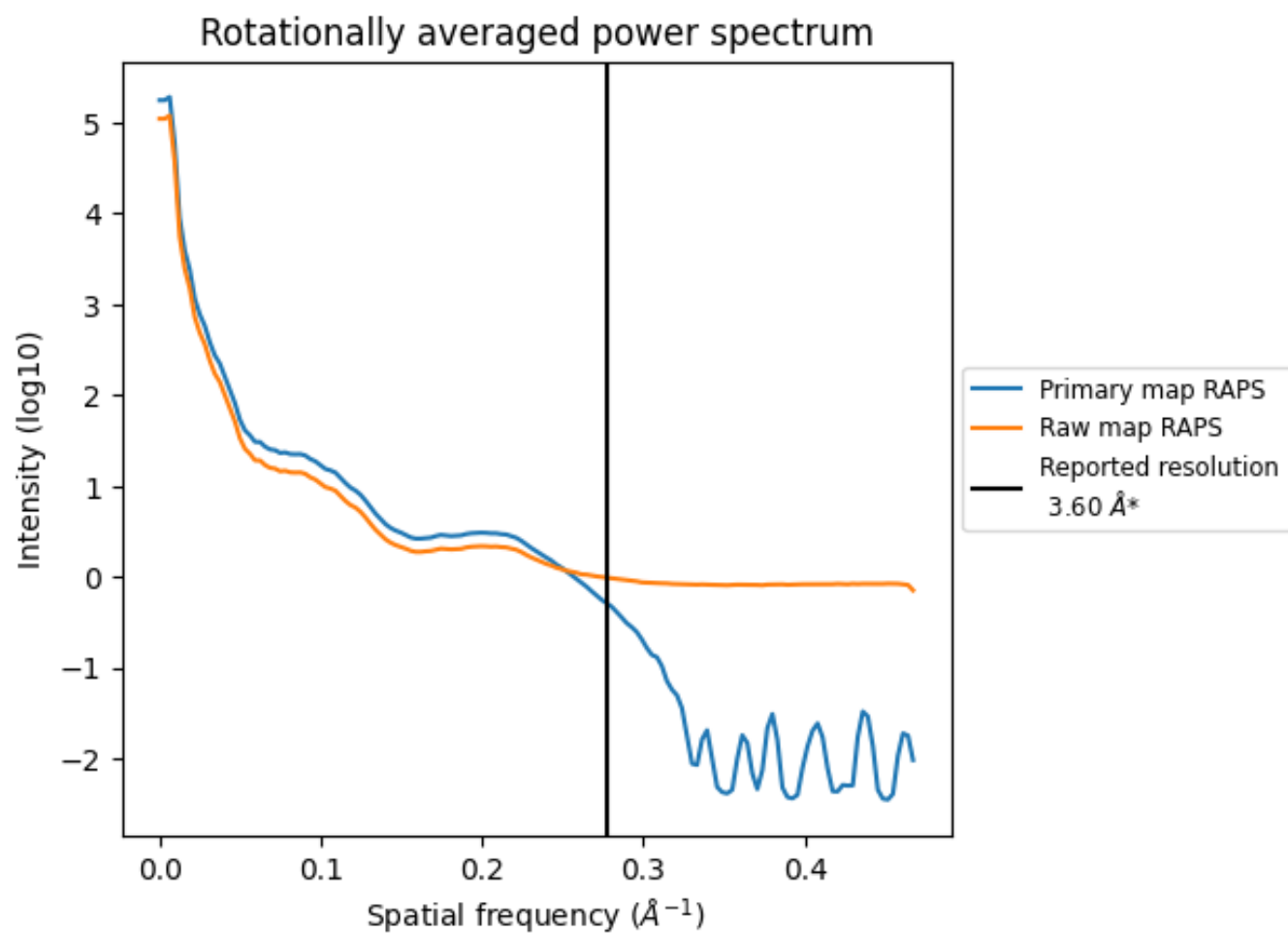
7.2 Volume estimate [i](#)



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 ⓘ

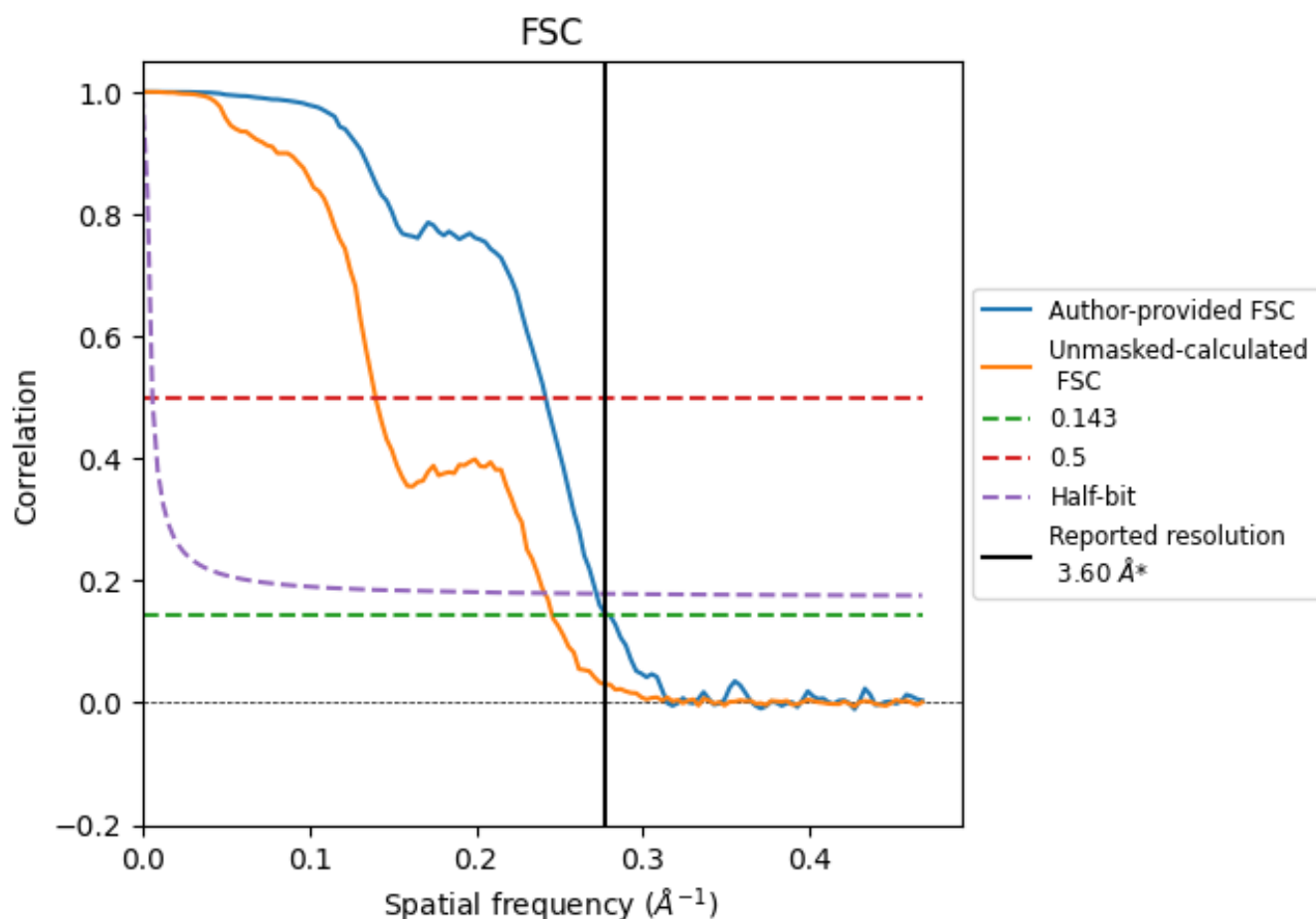


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

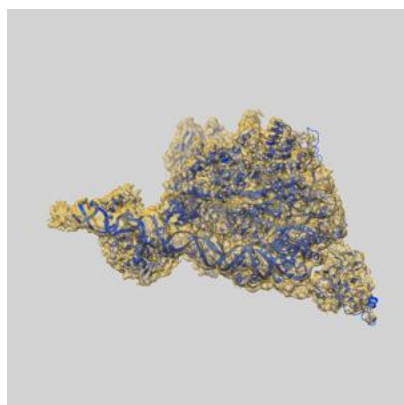
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.14	3.67
Unmasked-calculated*	4.07	7.15	4.15

*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 %

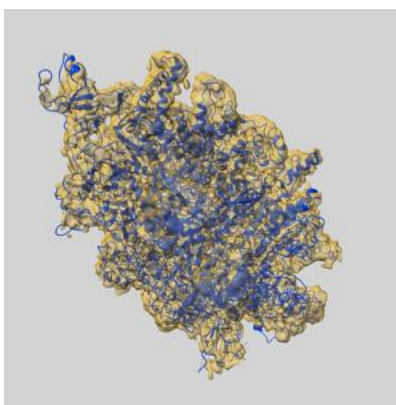
9 Map-model fit [i](#)

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](#).

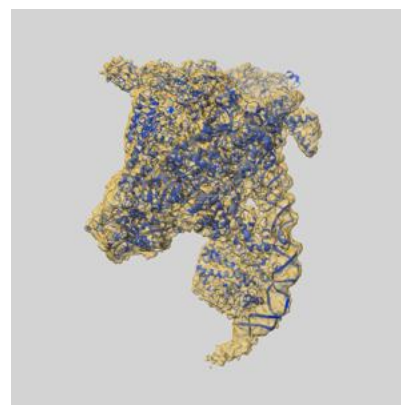
9.1 Map-model overlay [i](#)



X



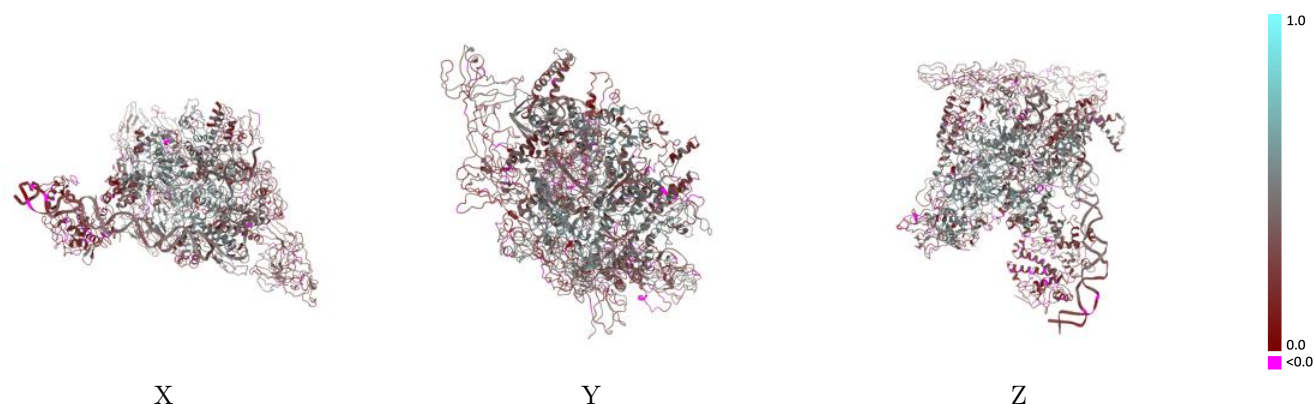
Y



Z

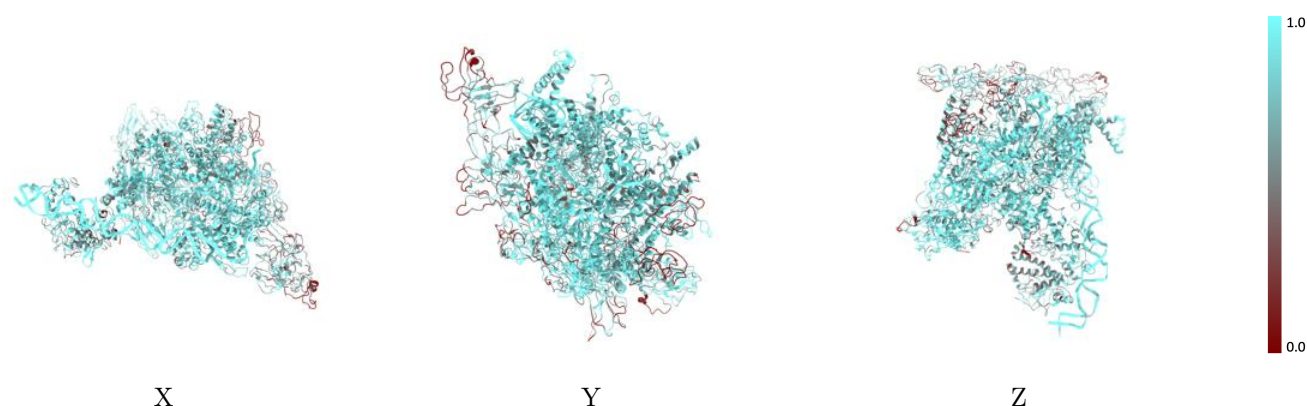
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



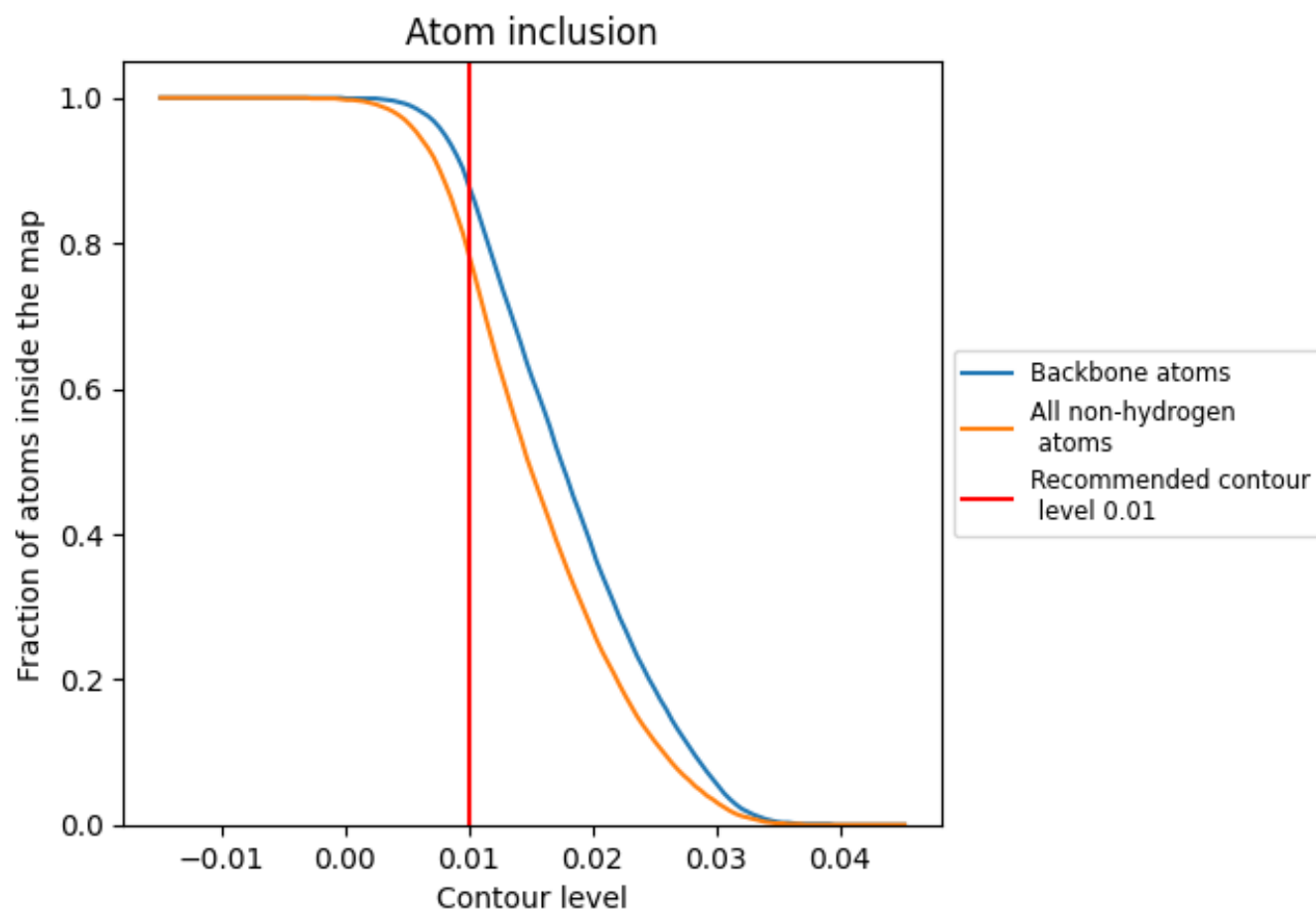
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

1.0

0.0

<0.0