



wwPDB EM Validation Summary Report ⓘ

Dec 7, 2022 – 11:50 AM JST

PDB ID : 6KF9
EMDB ID : EMD-9970
Title : Cryo-EM structure of Thermococcus kodakarensis RNA polymerase
Authors : Jun, S.-H.; Hyun, J.; Jeong, H.; Cha, J.S.; Kim, H.; Bartlett, M.S.; Cho, H.-S.;
Murakami, K.S.
Deposited on : 2019-07-07
Resolution : 3.79 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:

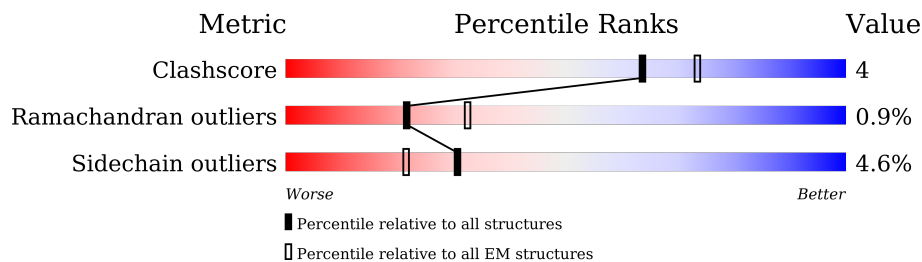
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	906	
2	B	1123	
3	C	391	
4	D	259	
5	E	190	
6	F	122	
7	H	82	
8	K	57	

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Mol	Chain	Length	Quality of chain
9	L	94	
10	N	65	
11	P	49	
12	G	185	
13	X	16	
14	Y	27	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 28232 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	900	7181	4535	1277	1330	39	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1114	8892	5616	1587	1652	37	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	388	3037	1920	525	582	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	257	2058	1325	340	389	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	181	1465	939	250	267	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	122	1020	654	169	193	4	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	115	ILE	-	expression tag	UNP Q5JI52
F	116	ASP	-	expression tag	UNP Q5JI52
F	117	GLU	-	expression tag	UNP Q5JI52
F	118	TYR	-	expression tag	UNP Q5JI52
F	119	ARG	-	expression tag	UNP Q5JI52
F	120	PRO	-	expression tag	UNP Q5JI52
F	121	LEU	-	expression tag	UNP Q5JI52
F	122	GLU	-	expression tag	UNP Q5JI52

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	76	Total	C	N	O	0	0
			627	408	105	114		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	56	Total	C	N	O	S	0	0
			433	284	75	73	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	94	Total	C	N	O	S	0	0
			775	493	134	146	2		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	65	Total	C	N	O	S	0	0
			529	340	89	94	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	44	Total	C	N	O	S	0	0
			352	221	70	57	4		

- Molecule 12 is a protein called Transcription factor E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	166	1386	881	228	267	10	0	0

- Molecule 13 is a DNA chain called DNA (5'-D(P*TP*CP*GP*GP*TP*AP*AP*TP*CP*A P*CP*GP*CP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	X	14	285	136	50	85	14	0	0

- Molecule 14 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	Y	9	185	88	35	53	9	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

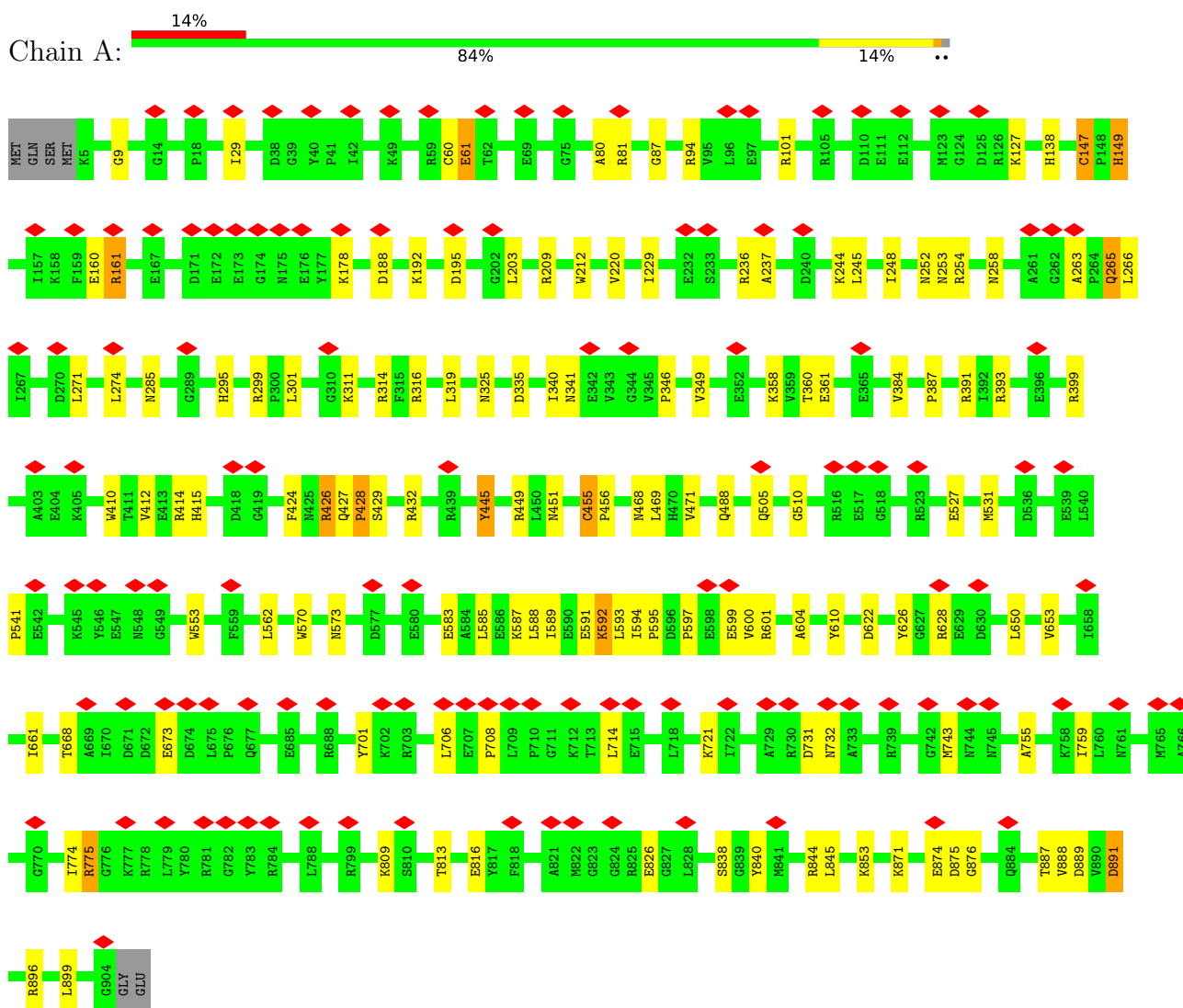
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
16	A	2	2	2	0
16	B	1	1	1	0
16	N	1	1	1	0
16	P	1	1	1	0
16	G	1	1	1	0

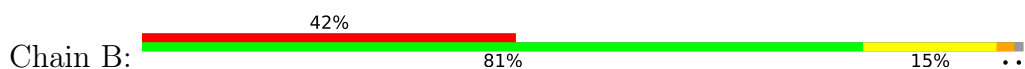
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

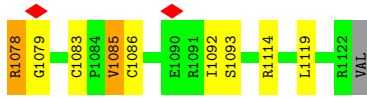
- Molecule 1: DNA-directed RNA polymerase subunit



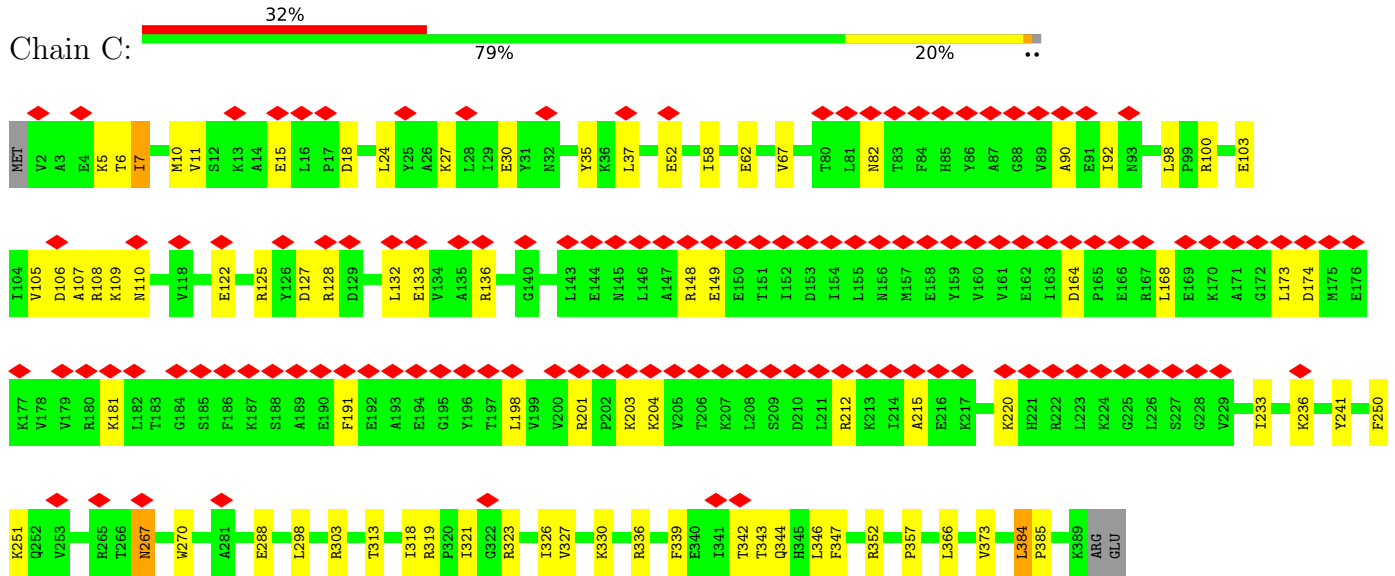
- Molecule 2: DNA-directed RNA polymerase subunit beta



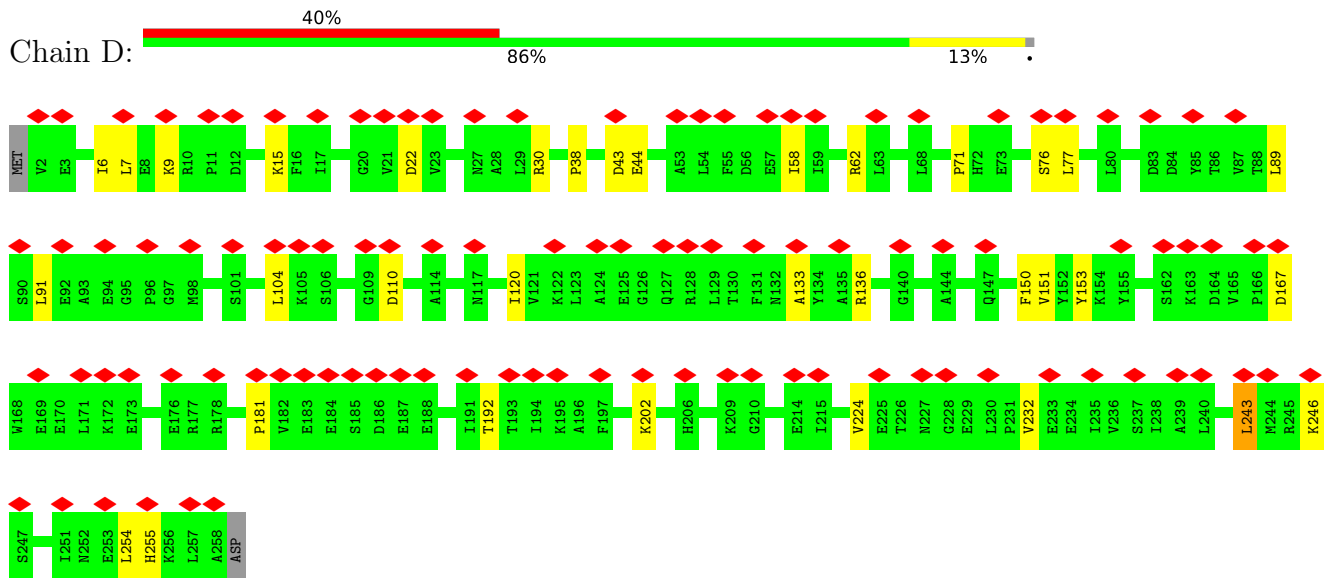
ME1	SER	ARG	GLY	VAL	THR	THR	E9	P10	T11	L12	T13	P14	D15	L16	L17	W18	L19	S23	K26	E27	K28	G29	F30	V31	R32	Q33	H34	L35	D36	N39	A40	D43	H44	G45	L46	Q47	V60	N51	E52	F53	G54	E55	V56	V57	P58	D59	I60	P61	M62	F63	K64	V65	K66			
F67	G68	K69	I70	I71	I72	F77	Q78	Q81	R84	P88	Y89	M90	R93	I94	R95	N96	L97	Y99	S100	A101	P102	L103	Y104	L105	E106	H107	I108	I109	V110	V111	N112	G113	H114	E115	Q116	K117	P118	V119	E120	V121	R122	I123	G124	E125	L126	P127	L130	K131	A203	K133	L137					
Y138	G139	L140	S141	D142	E143	E144	L145	K147	L148	P152	I161	E165	R166	V167	I168	V169	S170	E172	D173	R233	A234	L235	P176	N177	K178	T179	L180	V181	E182	R183	D184	E185	R186	Q187	N188	K189	V190	A191	R252	K193	V194	F195	S196	Y197	R198	H199	G200	A264	S265	L204	I205	S268	T269	Q270	E271	E272
R209	K210	K211	D212	G213	I214	L215	V216	V217	T218	I219	P220	V222	P223	K224	P225	V226	K227	F228	V229	M232	R233	A234	L235	G236	L237	L238	T239	D240	K241	E242	I243	V244	E245	A246	V247	S248	D249	D250	P251	R252	L253	F258	D259	M260	L261	E262	D263	A264	S265	L266	I267	S268	T269	Q270	E271	E272
A273	L274	D275	Y276	I277	G278	R279	L280	A281	L282	P283	G284	Q285	P286	E288	Y289	R290	L291	R292	R293	A294	E295	H296	L297	D299	N300	N301	L302	L303	F304	H305	K306	G307	V308	D309	P310	E311	N312	R313	R314	A315	K316	A317	Y318	Y319	M322	M323	A324	L325	E329	L332	G333	L334	R335	G336		
E337	D338	D339	K340	D341	H342	Y343	A344	N345	K346	R347	L348	A351	G352	D353	K356	L358	F359	R360	V361	A362	F363	L366	V367	K368	D369	M370	Q371	Y372	Q373	K374	T375	K376	T377	Q379	R380	K381	G382	E383	R384	Y385	T386	F387	E388	K389	L390	Q391	F393	V394	R395	N396	L398	R399				
P400	D401	V402	L403	S404	E405	R406	L407	E408	L411	G414	G418	G419	R420	T421	G422	V423	S424	Q425	L426	L427	D428	R429	N431	Y432	M433	L436	L439	R440	R441	R448	H452	F453	E454	A455	R456	D457	L458	H459	G460	A463	G464	E470	E473	C477	G478	N482	L483									
A484	L485	H486	T491	G492	L493	P494	E495	R496	E497	V498	R499	E500	K504	M505	G506	P509	L510	E511	E512	R514	P515	A516	P517	Y520	R521	V522	L528	N529	G530	T531	V532	E533	D534	G535	R536	K537	E540	R541	A544	D545	R546	R547	A548	G549	L551	S552	D553	V554	L555	N556						
V557	A558	L559	V560	E561	D562	E564	V565	R566	E567	V568	D573	R576	R579	L581	I582	V583	V584	E585	N586	G587	K588	L591	T592	R593	E594	R600	N601	G602	T603	L604	T605	D608	L609	M612	G613	V614	L615	E616	V617	E622	E623	E624	N625	A629	T630	M631	P632	W633								
E634	V635	T636	E637	L642	M645	P646	A647	L650	G651	I652	P653	A654	S655	Y659	P660	E661	H662	R667	N668	G671	A672	E674	K675	R676	K677	D679	D680	L681	G682	M683	A684	R687	L688	D691	T692	R693	M697	H698	V699	L704	V705	N706	S707	R708	K711	A712	E716									
D717	Q722	N723	F724	V725	V726	N735	D738	A739	V740	I741	I742	N743	K744	R745	S746	E748	R749	G750	L751	A752	E761	A762	E764	K765	R766	K772	D773	M774	F775	E776	S779	F780	N781	I782	G783	G784	Y785	L786	G787	E788	K789	H793	D797	G798	V870	L878	G879	D880	S884							
D810	V811	L812	R815	T816	S817	P818	P819	R820	F821	I822	E823	E824	Q825	S826	S827	L828	G829	D911	M831	V832	L833	Q834	G835	R836	R837	E838	R844	E847	K848	V851	D852	K853	V854	L855	V856	E858	T859	G860	D861	G862	H863	K864	L865	V868	T869	V870	L878	G879	D880	S884						
R885	H886	G887	Q888	L894	P897	Q898	E899	P902	W903	T904	E905	S906	G907	I908	V909	P910	D911	L912	I919	V925	G926	Q927	L928	I929	I932	K935	L939	T940	G941	R942	R943	V944	D945	G946	I950	G951	E952	P953	E954	E955	K956	L957	R958	K959	E960	L961	E962	E963	L964	G965						
F966	K967	H968	S969	G970	R971	E972	H974	Y975	R976	G977	Y978	R981	R982	L983	E984	A985	D986	Y992	Y993	Y994	H998	H999	R1008	S1009	L1010	G1011	V1015	L1016	T1017	R1024	E1027	G1028	G1029	L1030	R1031	E1036	R1052	E1056	S1057	E954	D1058	C1065	E1066	E1074	D1075	K1076	R1077									



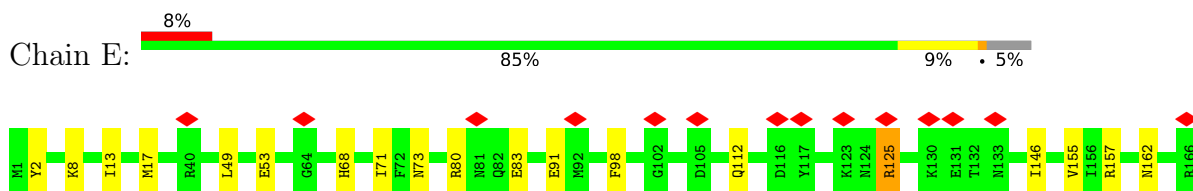
- Molecule 3: DNA-directed RNA polymerase subunit A''

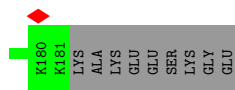


- Molecule 4: DNA-directed RNA polymerase subunit D

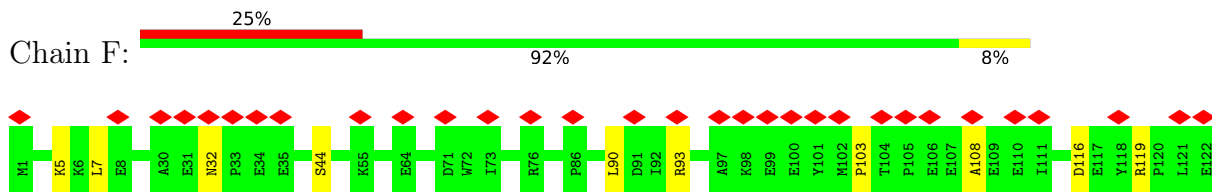


- Molecule 5: DNA-directed RNA polymerase, subunit E

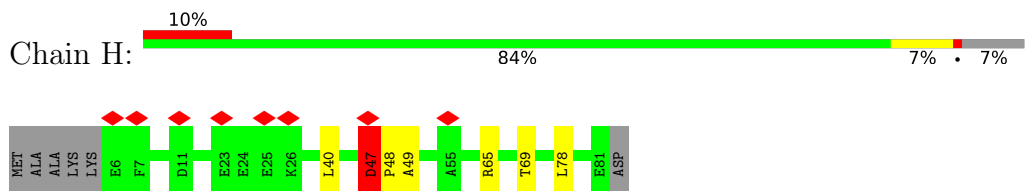




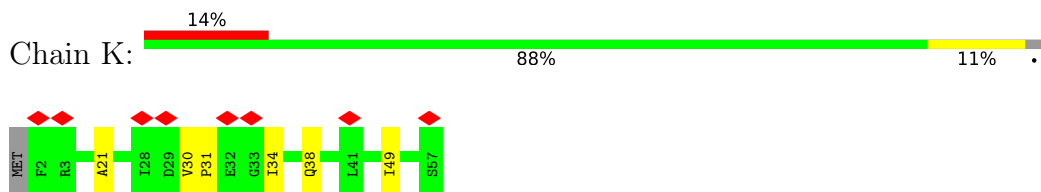
• Molecule 6: DNA-directed RNA polymerase, subunit F



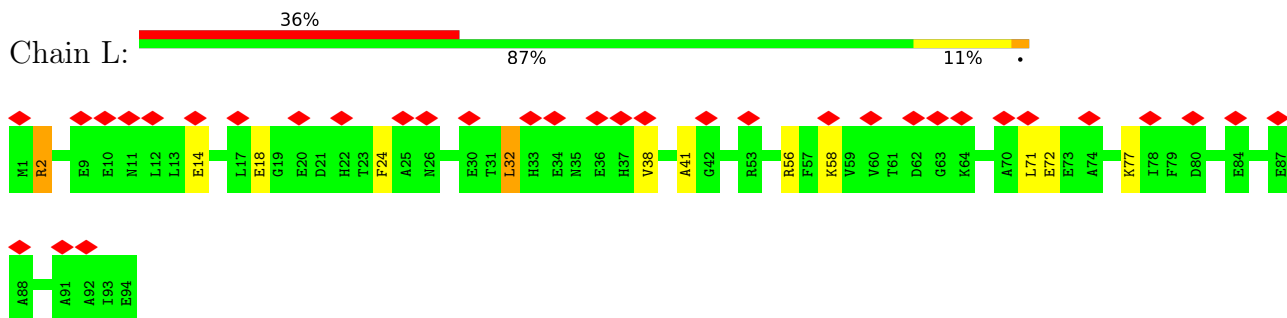
• Molecule 7: DNA-directed RNA polymerase subunit H



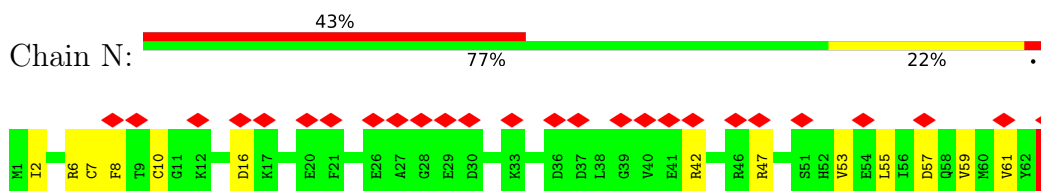
• Molecule 8: DNA-directed RNA polymerase subunit K



• Molecule 9: DNA-directed RNA polymerase subunit L

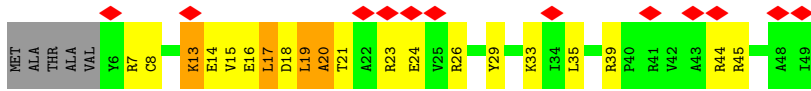


• Molecule 10: DNA-directed RNA polymerase subunit N

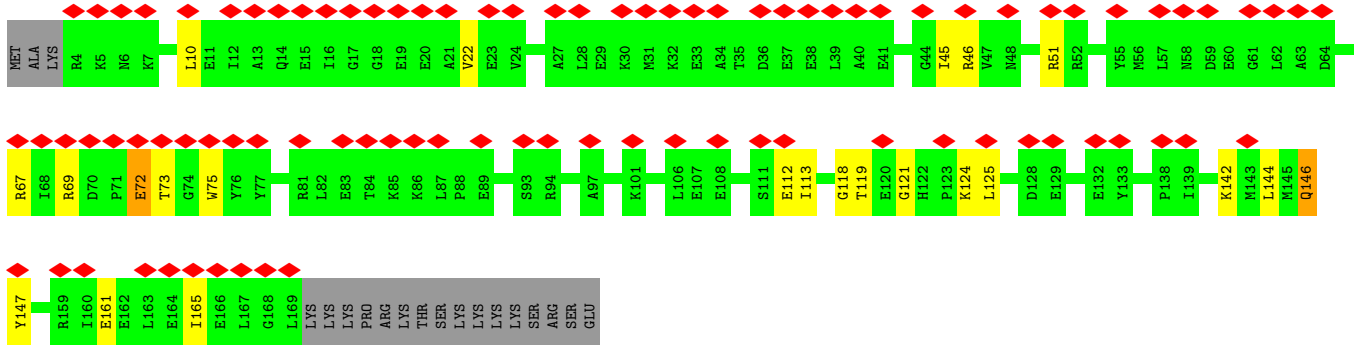
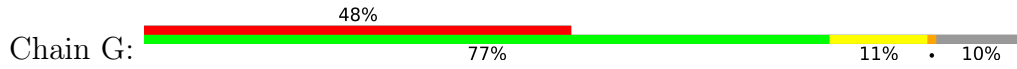


• Molecule 11: DNA-directed RNA polymerase subunit P

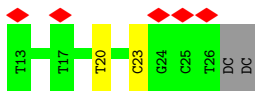
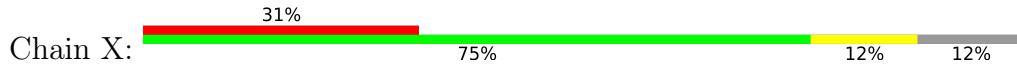




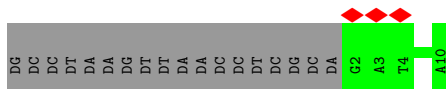
• Molecule 12: Transcription factor E



• Molecule 13: DNA (5'-D(P*TP*CP*GP*GP*TP*AP*AP*TP*CP*AP*CP*GP*CP*TP*CP*C)-3')



• Molecule 14: DNA (27-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	312092	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 ($e^-/\text{\AA}^2$)	35.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.966	Depositor
Minimum map value	-0.803	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	246.4, 246.4, 246.4	wwPDB
Map dimensions	176, 176, 176	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	1/7324 (0.0%)	0.68	1/9885 (0.0%)
2	B	0.40	0/9070	0.72	9/12256 (0.1%)
3	C	0.37	0/3077	0.71	3/4156 (0.1%)
4	D	0.38	0/2103	0.65	0/2848
5	E	0.34	1/1491 (0.1%)	0.53	0/2008
6	F	0.26	0/1040	0.54	0/1399
7	H	0.38	0/641	0.73	1/866 (0.1%)
8	K	0.36	0/441	0.60	0/598
9	L	0.33	0/790	0.62	0/1066
10	N	0.48	0/538	0.76	0/723
11	P	0.42	0/357	1.01	3/477 (0.6%)
12	G	0.30	0/1409	0.56	0/1890
13	X	0.88	0/318	1.22	2/488 (0.4%)
14	Y	0.65	0/207	1.01	0/317
All	All	0.40	2/28806 (0.0%)	0.69	19/38977 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	3
3	C	0	6
7	H	0	1
8	K	0	2
11	P	0	1
12	G	0	3
All	All	0	19

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	125	ARG	CA-CB	6.06	1.67	1.53
1	A	562	LEU	C-N	-5.26	1.22	1.34

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	47	ASP	CB-CG-OD1	8.36	125.82	118.30
2	B	12	LEU	C-N-CA	6.92	139.01	121.70
13	X	23	DC	O4'-C1'-N1	6.92	112.84	108.00
2	B	1078	ARG	NE-CZ-NH1	6.34	123.47	120.30
13	X	20	DT	O4'-C1'-N1	6.16	112.31	108.00

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	GLN	Peptide
1	A	455	CYS	Peptide
1	A	874	GLU	Peptide
2	B	10	PRO	Peptide
2	B	704	LEU	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	A	7181	0	7249	73	0
2	B	8892	0	8950	93	0
3	C	3037	0	3151	38	0
4	D	2058	0	2068	20	0
5	E	1465	0	1503	9	0
6	F	1020	0	1024	5	0
7	H	627	0	642	3	0
8	K	433	0	466	3	0
9	L	775	0	770	9	0
10	N	529	0	543	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	P	352	0	376	9	0
12	G	1386	0	1382	12	0
13	X	285	0	159	0	0
14	Y	185	0	102	0	0
15	A	1	0	0	0	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	G	1	0	0	0	0
16	N	1	0	0	0	0
16	P	1	0	0	0	0
All	All	28232	0	28385	243	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 4.

The worst 5 of 243 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)
3:C:107:ALA:HB1	3:C:270:TRP:HE1	1.53	0.73
1:A:597:PRO:HA	1:A:601:ARG:HD2	1.72	0.72
1:A:445:TYR:HB2	1:A:449:ARG:HH22	1.58	0.67
1:A:203:LEU:HD21	3:C:352:ARG:HH21	1.61	0.65
10:N:7:CYS:SG	10:N:8:PHE:N	2.70	0.65

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	898/906 (99%)	750 (84%)	140 (16%)	8 (1%)	17	54
2	B	1112/1123 (99%)	940 (84%)	159 (14%)	13 (1%)	13	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	386/391 (99%)	309 (80%)	74 (19%)	3 (1%)	19	57
4	D	255/259 (98%)	242 (95%)	12 (5%)	1 (0%)	34	70
5	E	179/190 (94%)	166 (93%)	13 (7%)	0	100	100
6	F	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
7	H	74/82 (90%)	63 (85%)	10 (14%)	1 (1%)	11	46
8	K	54/57 (95%)	46 (85%)	8 (15%)	0	100	100
9	L	92/94 (98%)	82 (89%)	10 (11%)	0	100	100
10	N	63/65 (97%)	54 (86%)	8 (13%)	1 (2%)	9	44
11	P	42/49 (86%)	27 (64%)	14 (33%)	1 (2%)	6	37
12	G	164/185 (89%)	148 (90%)	14 (8%)	2 (1%)	13	50
All	All	3439/3523 (98%)	2937 (85%)	472 (14%)	30 (1%)	21	54

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	593	LEU
2	B	432	TYR
2	B	819	PRO
1	A	604	ALA
1	A	888	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	774/779 (99%)	741 (96%)	33 (4%)	29	58
2	B	961/969 (99%)	904 (94%)	57 (6%)	19	51
3	C	331/334 (99%)	314 (95%)	17 (5%)	24	54
4	D	226/228 (99%)	222 (98%)	4 (2%)	59	77
5	E	160/167 (96%)	156 (98%)	4 (2%)	47	70
6	F	107/107 (100%)	106 (99%)	1 (1%)	78	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	68/72 (94%)	67 (98%)	1 (2%)	65	81
8	K	45/46 (98%)	45 (100%)	0	100	100
9	L	81/81 (100%)	79 (98%)	2 (2%)	47	70
10	N	59/59 (100%)	54 (92%)	5 (8%)	10	40
11	P	37/40 (92%)	29 (78%)	8 (22%)	1	7
12	G	148/166 (89%)	143 (97%)	5 (3%)	37	64
All	All	2997/3048 (98%)	2860 (95%)	137 (5%)	31	56

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	32	ASN
10	N	42	ARG
11	P	29	TYR
2	B	289	TYR
2	B	288	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	19	ASN
3	C	267	ASN
3	C	124	HIS
3	C	344	GLN
1	A	732	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

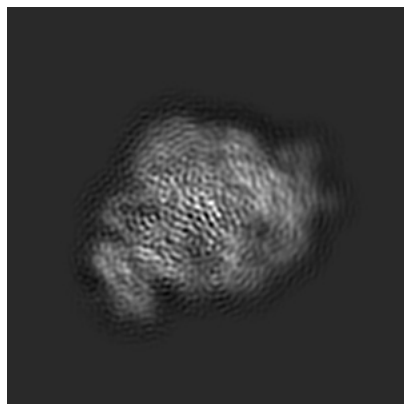
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9970. These allow visual inspection of the internal detail of the map and identification of artifacts.

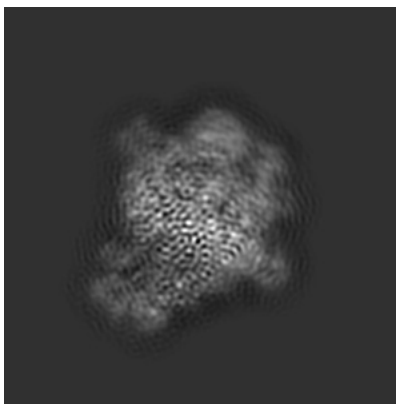
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

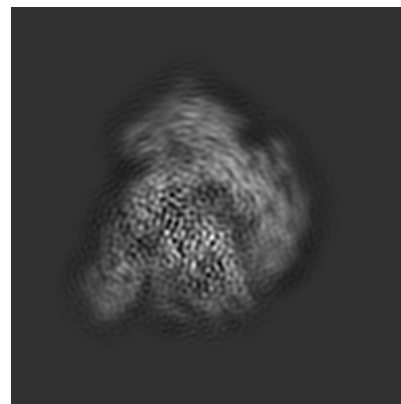
6.1.1 Primary map



X

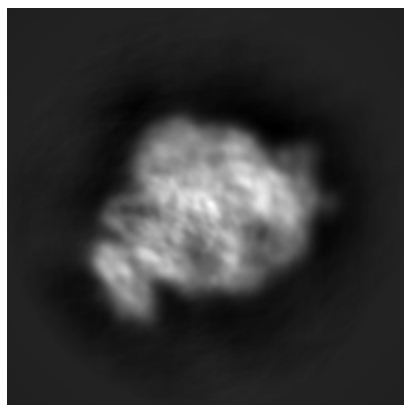


Y

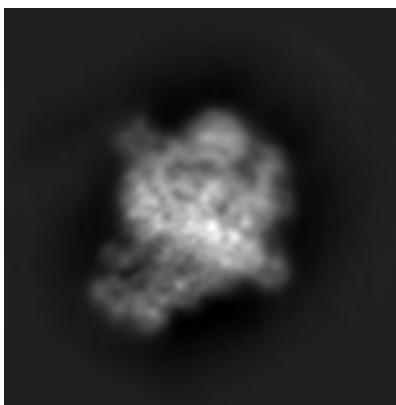


Z

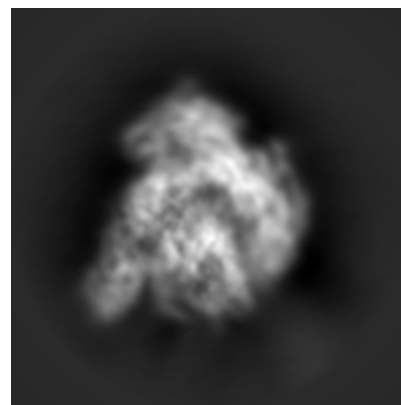
6.1.2 Raw map



X



Y

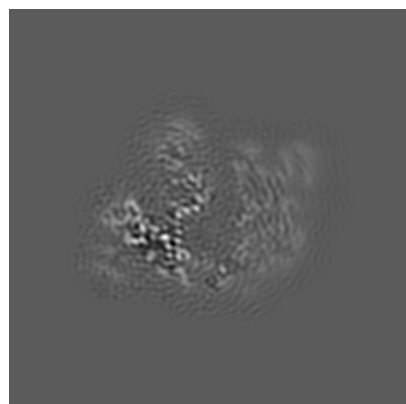


Z

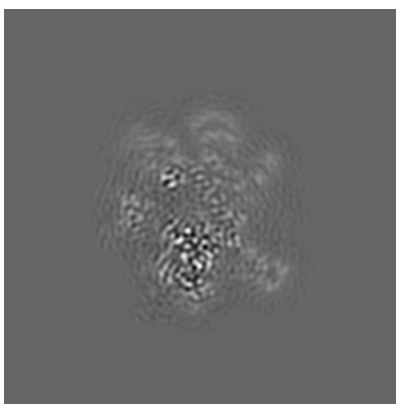
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

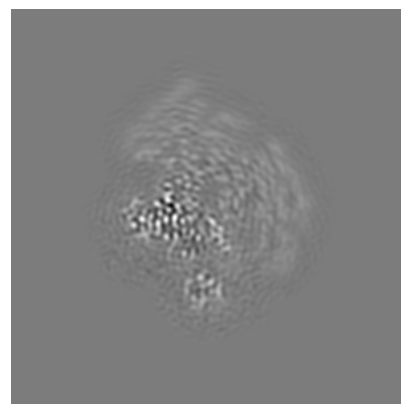
6.2.1 Primary map



X Index: 88

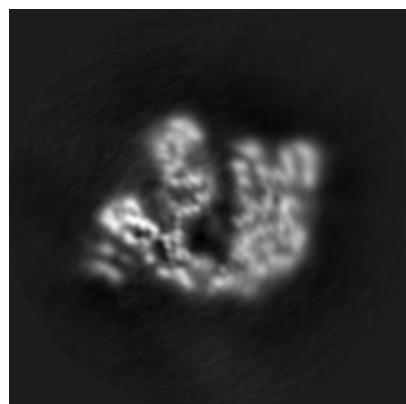


Y Index: 88

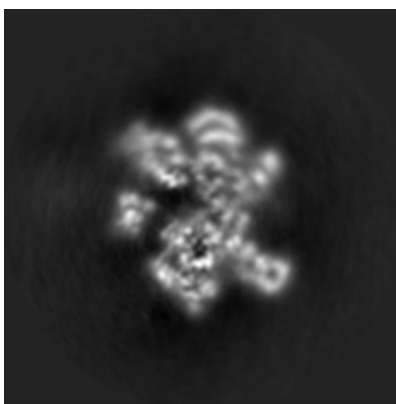


Z Index: 88

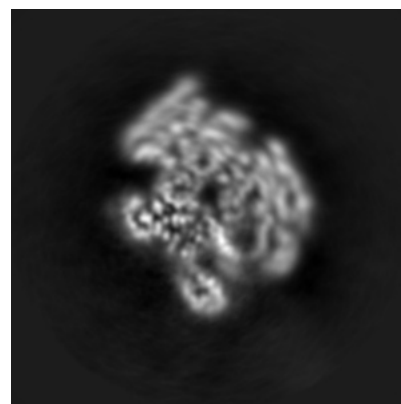
6.2.2 Raw map



X Index: 88



Y Index: 88

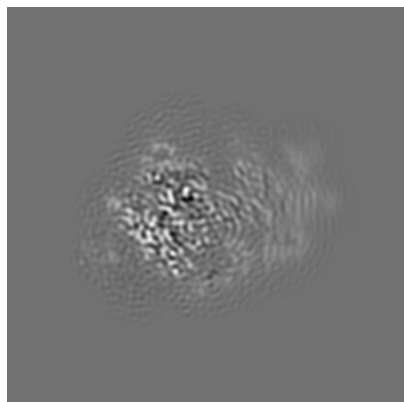


Z Index: 88

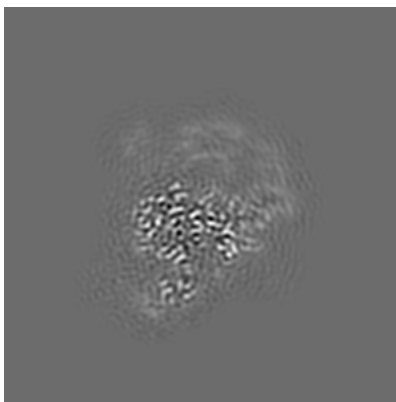
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

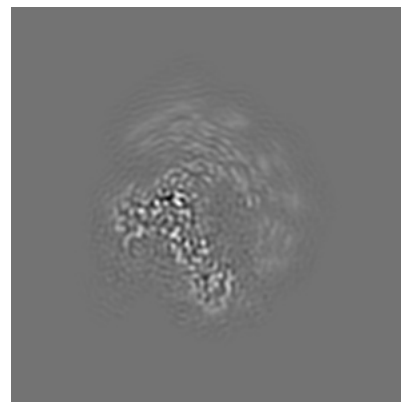
6.3.1 Primary map



X Index: 80

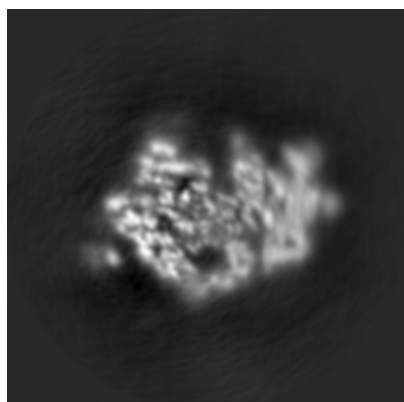


Y Index: 72

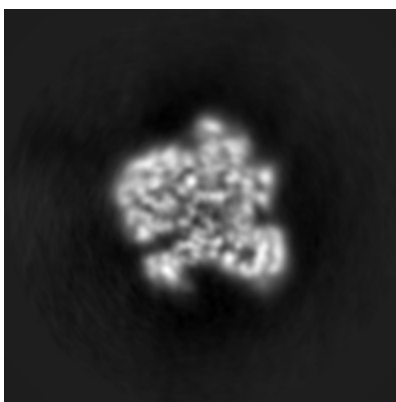


Z Index: 83

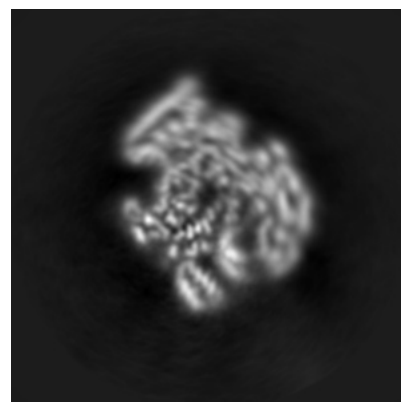
6.3.2 Raw map



X Index: 80



Y Index: 100

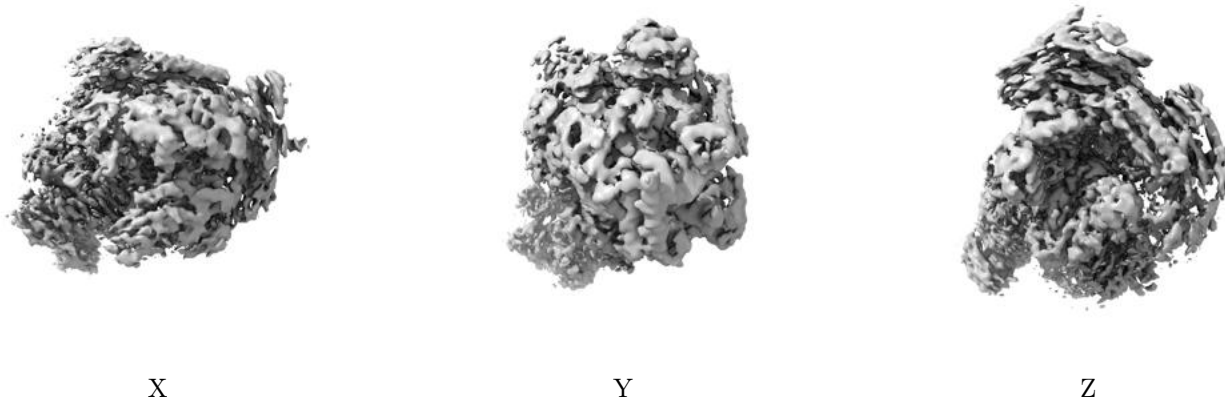


Z Index: 91

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

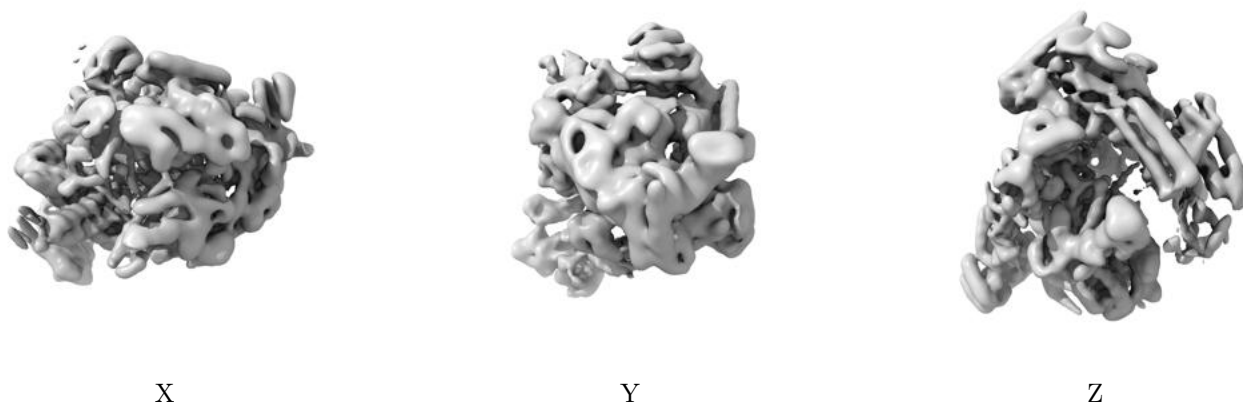
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

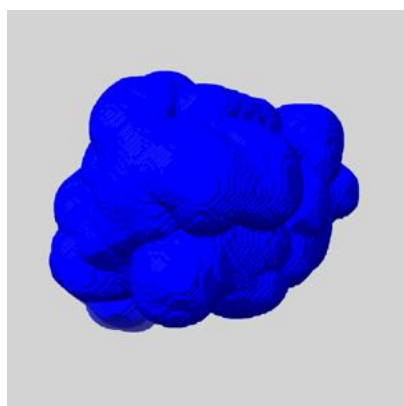
6.5 Mask visualisation [i](#)

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

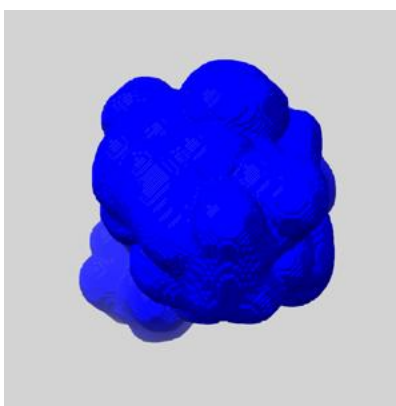
A mask typically either:

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

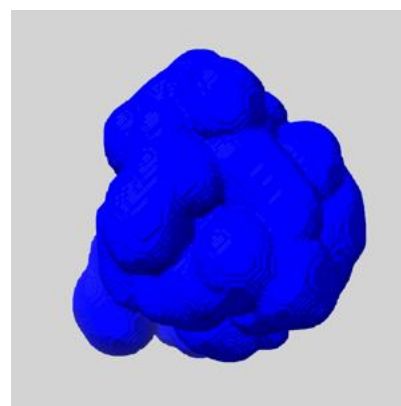
6.5.1 emd_9970_msk_1.map [i](#)



X



Y

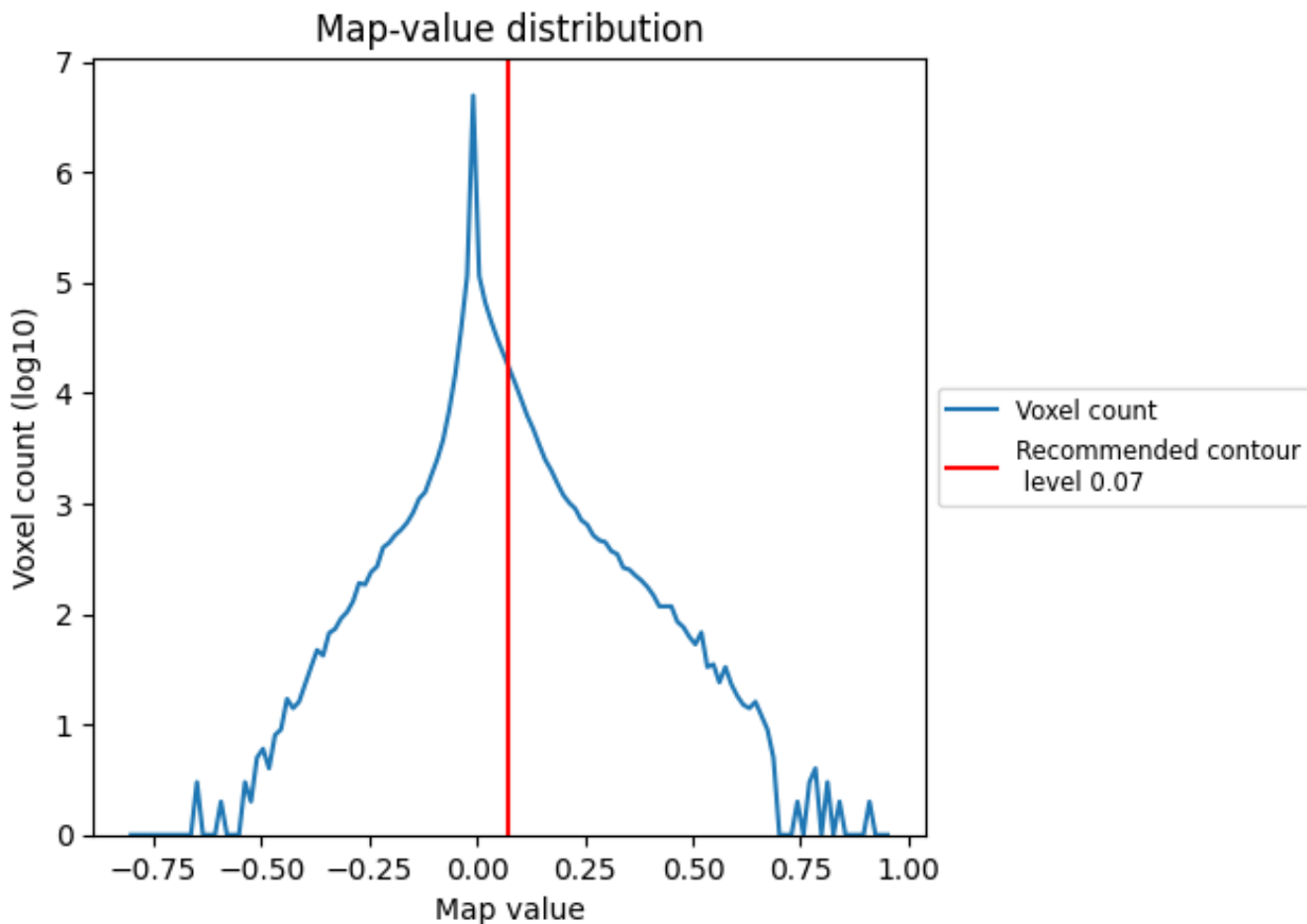


Z

7 Map analysis [i](#)

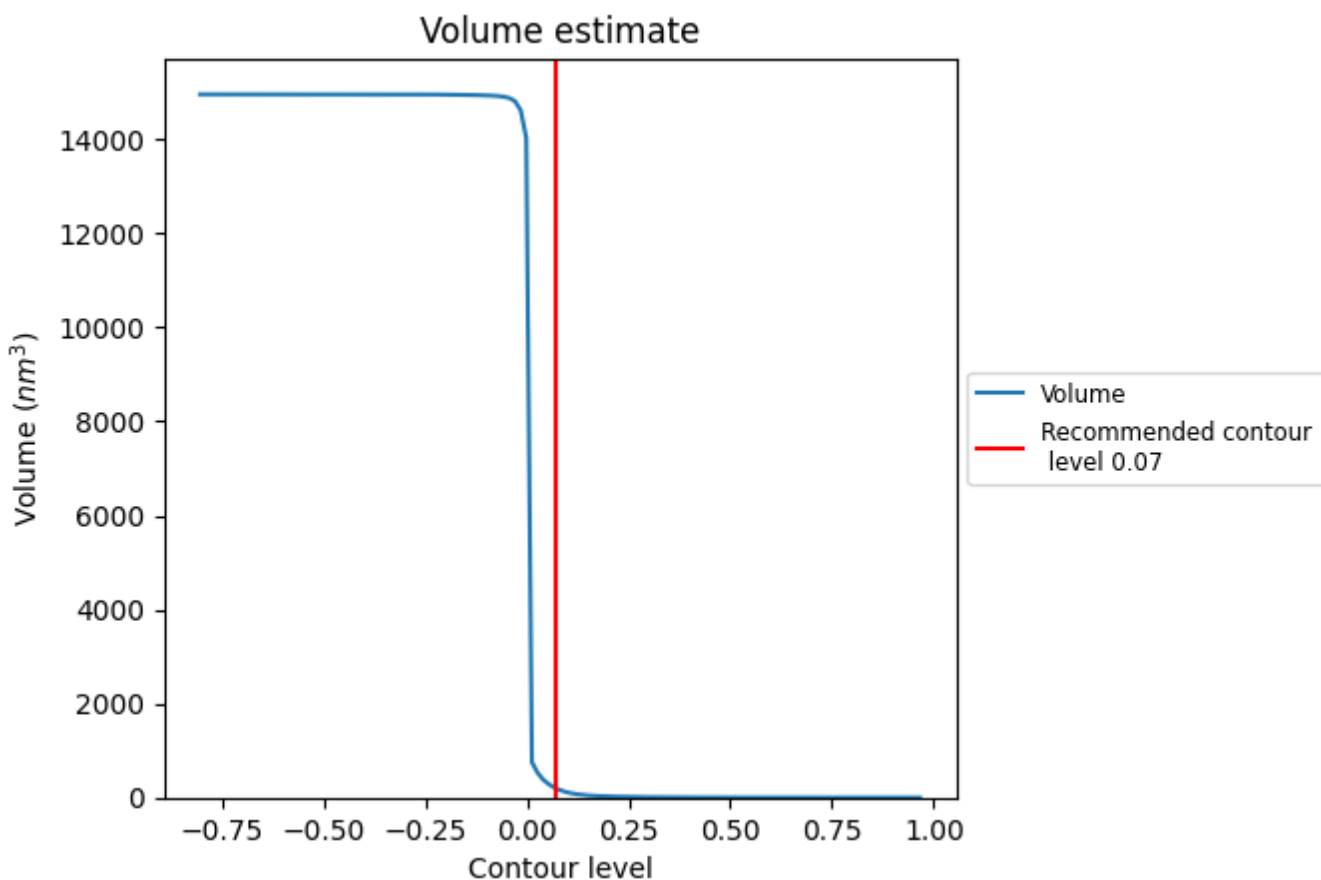
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

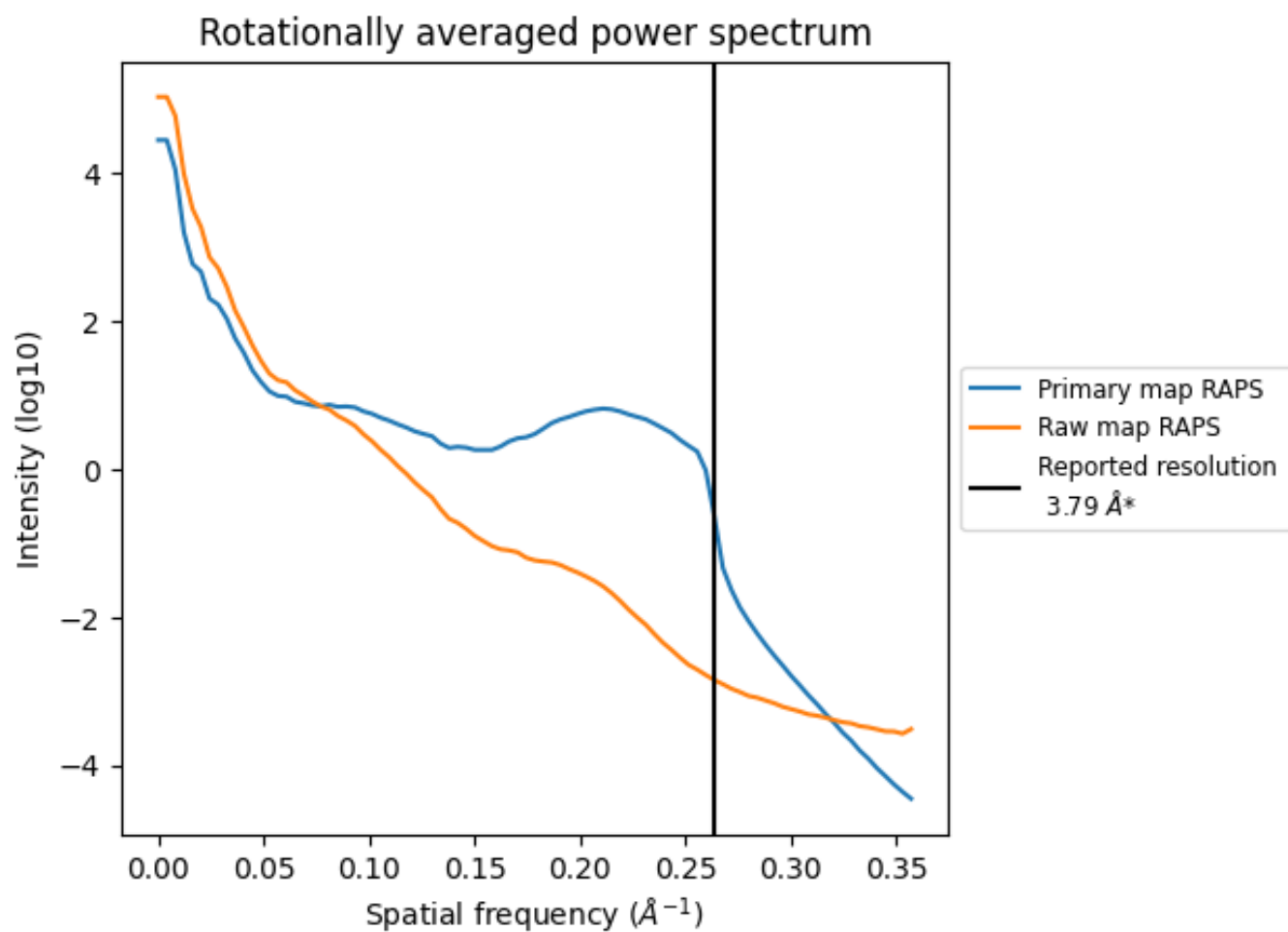
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 183 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 i

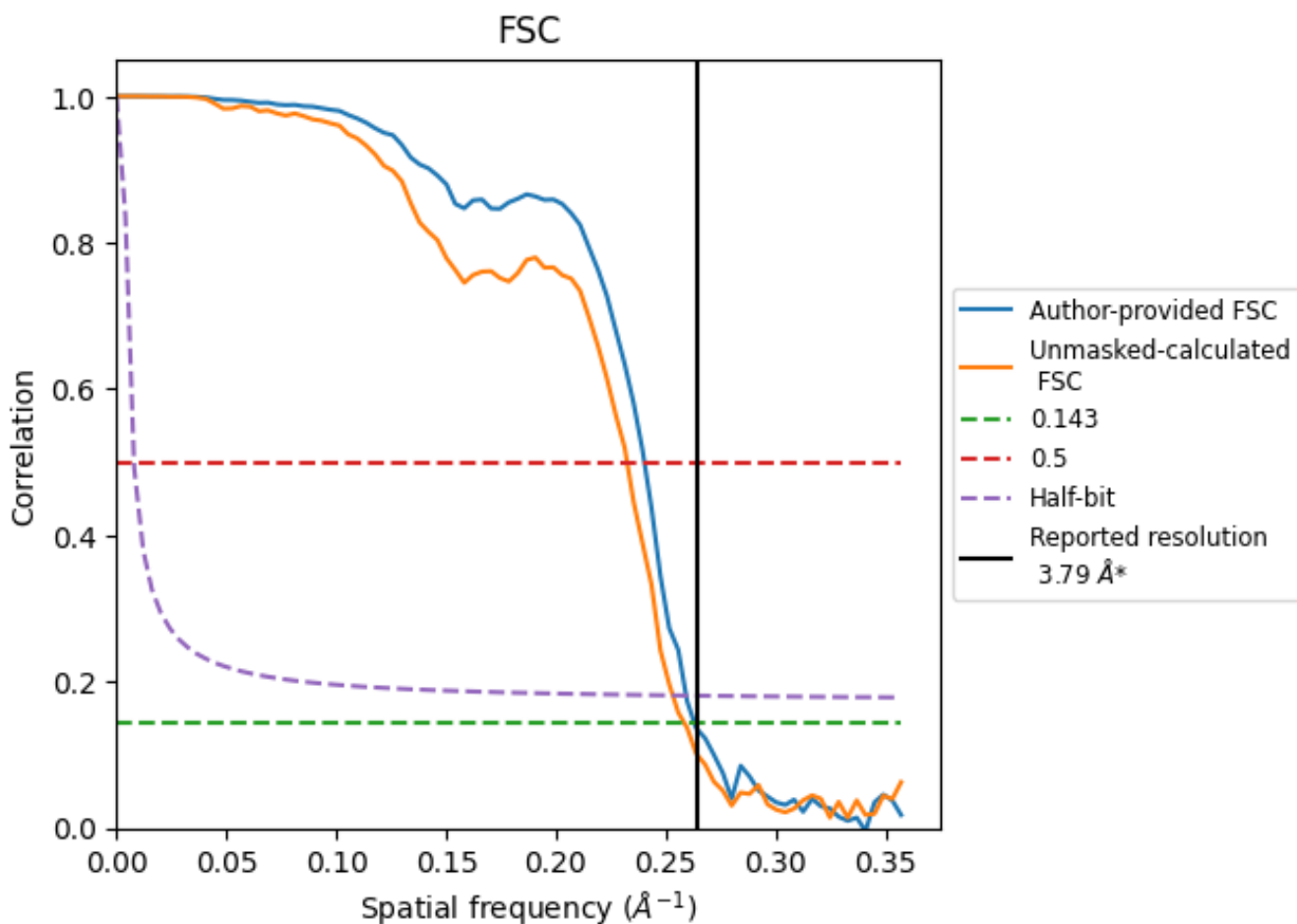


*Reported resolution corresponds to spatial frequency of 0.264 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.264 Å⁻¹

8.2 Resolution estimates [i](#)

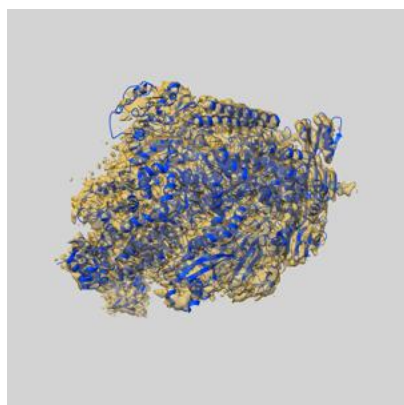
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.79	-	-
Author-provided FSC curve	3.80	4.16	3.86
Unmasked-calculated*	3.87	4.30	3.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

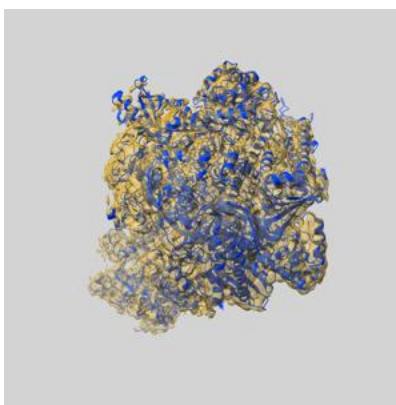
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9970 and PDB model 6KF9. Per-residue inclusion information can be found in section 3 on page 7.

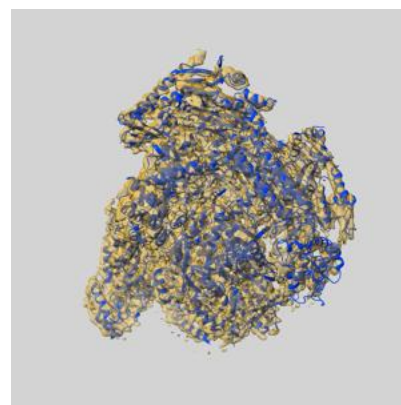
9.1 Map-model overlay [i](#)



X



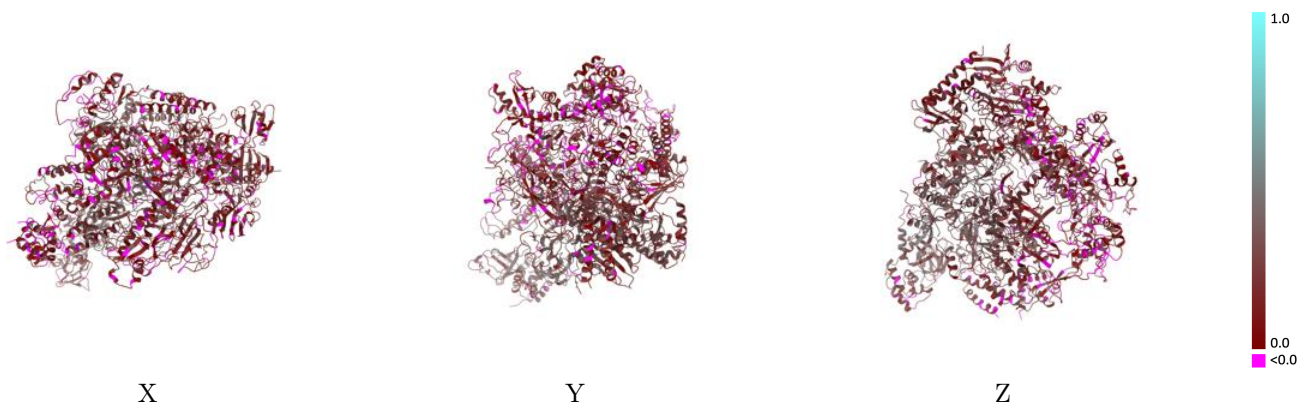
Y



Z

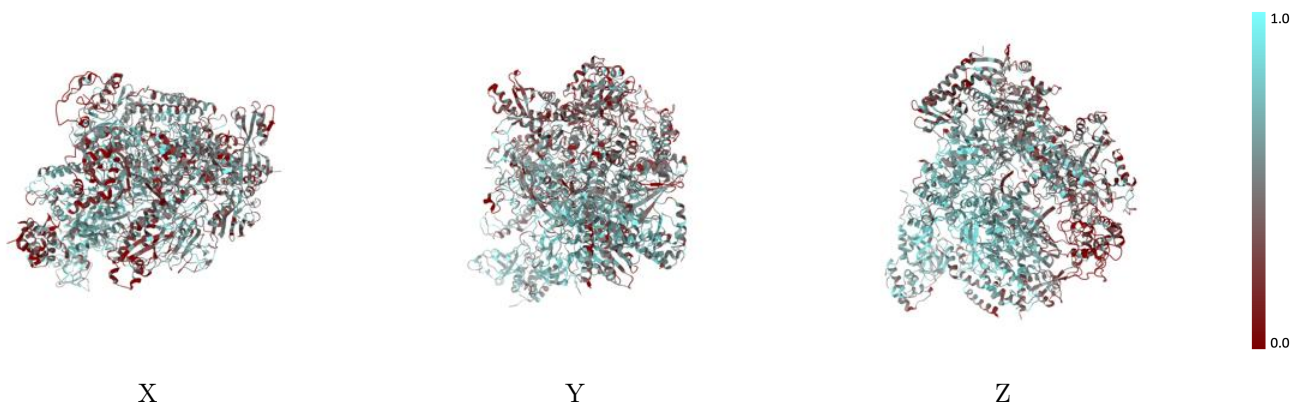
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



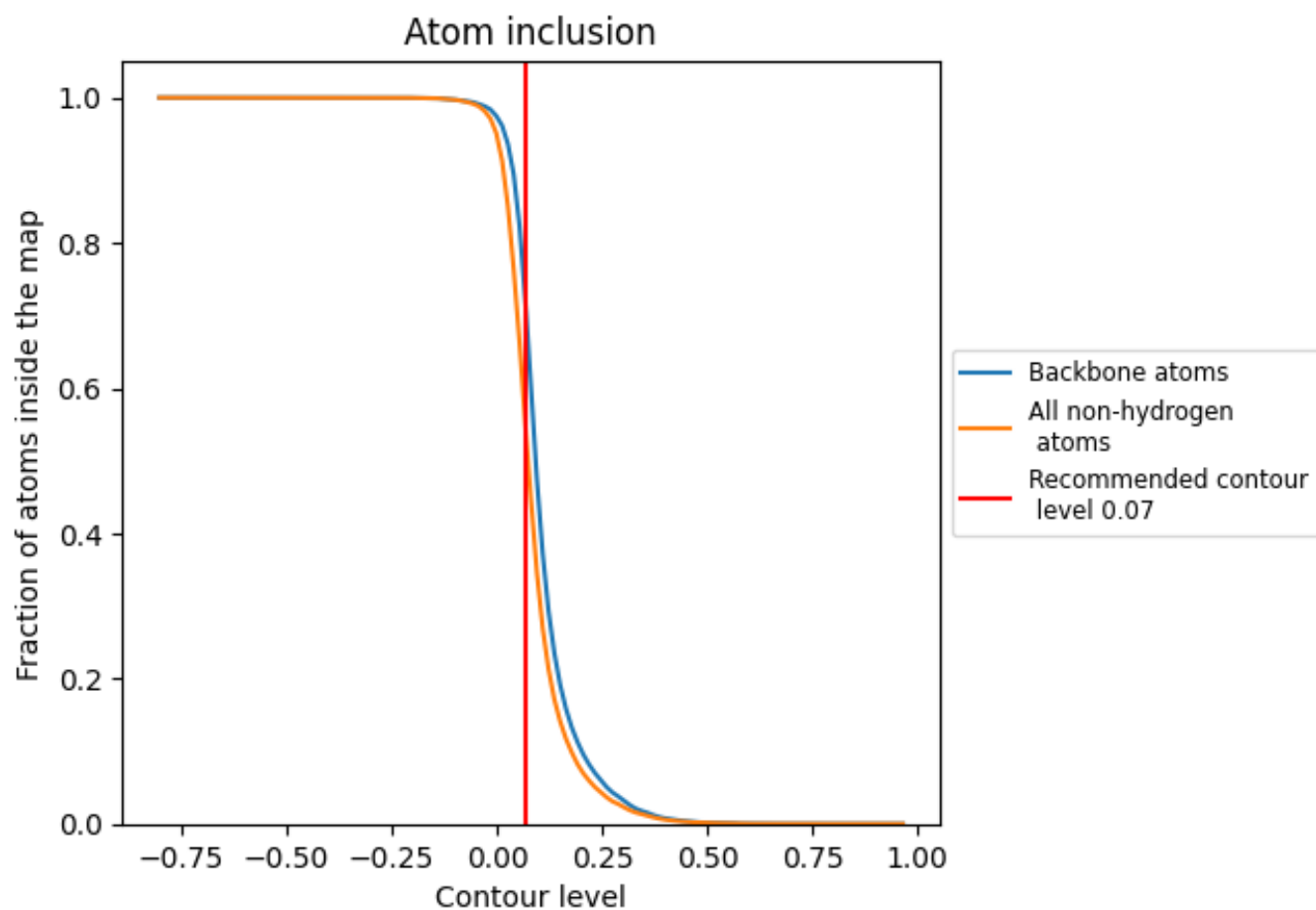
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 53% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5311	 0.2010
A	 0.6380	 0.2440
B	 0.4547	 0.1610
C	 0.5018	 0.2160
D	 0.4523	 0.1580
E	 0.6888	 0.3080
F	 0.5582	 0.2220
G	 0.3984	 0.1280
H	 0.7103	 0.2920
K	 0.7156	 0.3140
L	 0.5079	 0.2170
N	 0.4291	 0.1190
P	 0.5268	 0.1490
X	 0.4561	 0.0980
Y	 0.4865	 0.1520

