



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 10:05 AM UTC

PDB ID : 7MK9 / pdb_00007mk9
EMDB ID : EMD-23887
Title : Complex structure of trailing EC of EC+EC (trailing EC-focused)
Authors : Yang, C.; Murakami, K.
Deposited on : 2021-04-22
Resolution : 3.54 Å(reported)
Based on initial models : 3PO2, 5C4J

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:

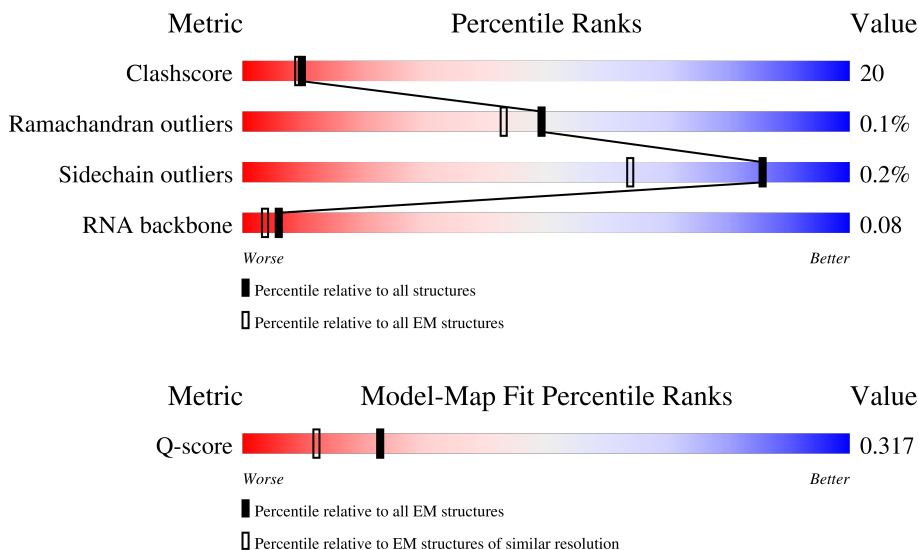
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.54 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	12891 (3.04 - 4.04)

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

Mol	Chain	Length	Quality of chain
1	N	40	
2	O	40	
3	A	1733	

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Mol	Chain	Length	Quality of chain
4	B	1224	
5	C	318	
6	D	221	
7	E	215	
8	F	155	
9	G	171	
10	H	146	
11	I	122	
12	J	70	
13	K	120	
14	L	70	
15	R	15	
16	Q	735	
17	M	400	

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 36122 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 (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	N	40	822	393	162	227	40	0	0

- Molecule 2 is a DNA chain called DNA (40-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	O	40	827	396	141	250	40	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	1425	11167	7036	1948	2121	62	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	1166	9227	5823	1619	1729	56	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	265	2086	1312	347	414	13	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	168	1331	822	237	270	2	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	E	214	1752	1111	309	321	11	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I,II,and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	F	87	705	451	119	132	3	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	G	171	1335	858	221	248	8	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	H	135	1080	679	182	214	5	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	I	114	927	571	168	178	10	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerases II subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	J	66	540	345	94	95	6	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	K	115	924	593	157	172	2	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerases II subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 15 is a RNA chain called RNA (5'-R(P*UP*CP*GP*AP*GP*AP*GP*GP*AP*U P*CP*CP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	15	Total	C	N	O	P	0	0
			312	141	56	100	15		

- Molecule 16 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	214	Total	C	N	O	S	0	0
			1619	1017	297	299	6		

- Molecule 17 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	135	Total	C	N	O	S	0	0
			1106	694	197	210	5		

- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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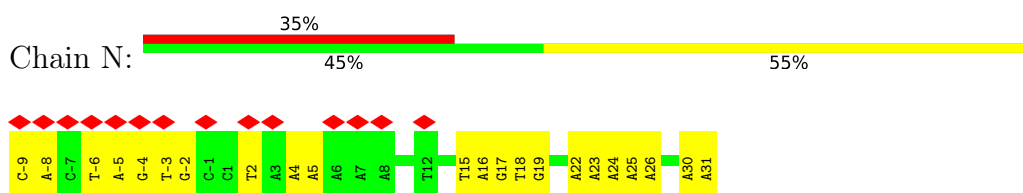
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
19	R	1	1	1	0

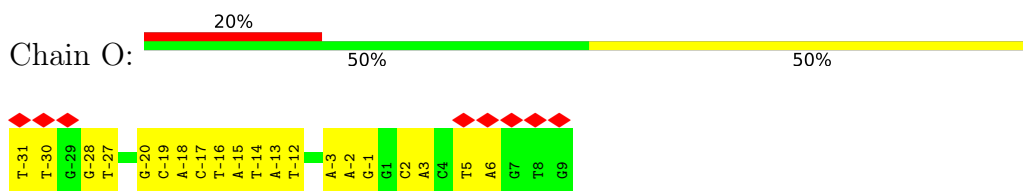
3 Residue-property plots [i](#)

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

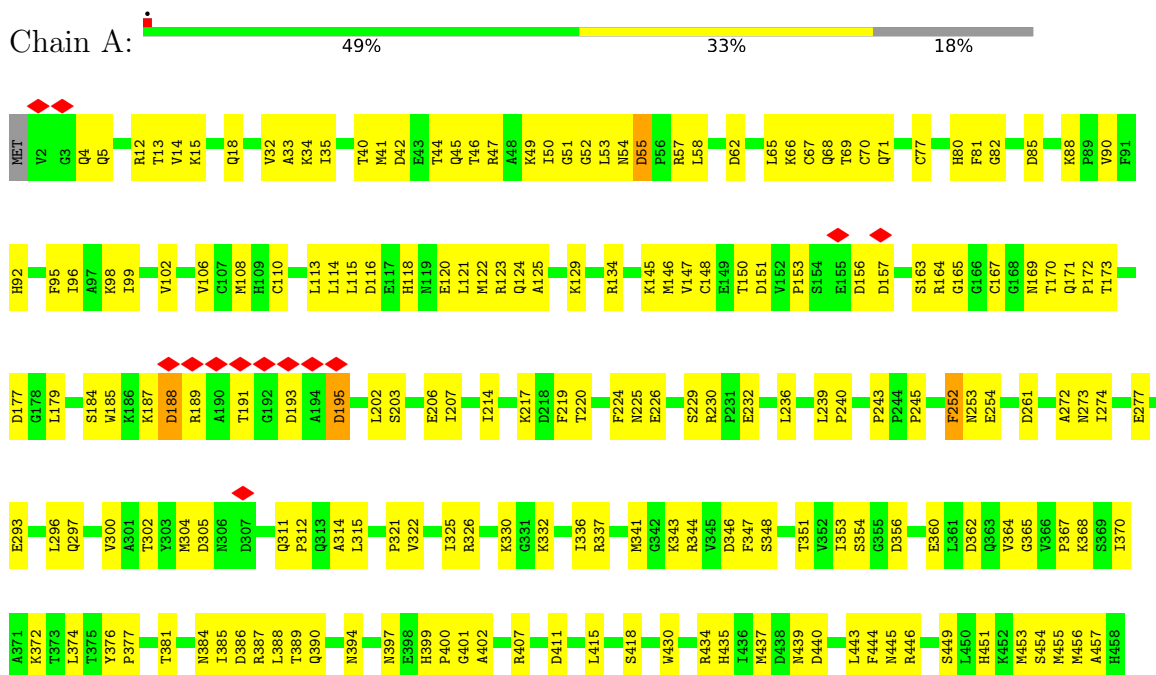
- Molecule 1: DNA (40-MER)



- Molecule 2: DNA (40-MER)

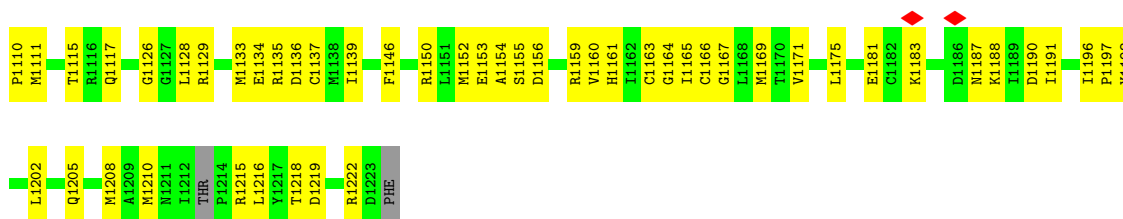


- Molecule 3: DNA-directed RNA polymerase subunit



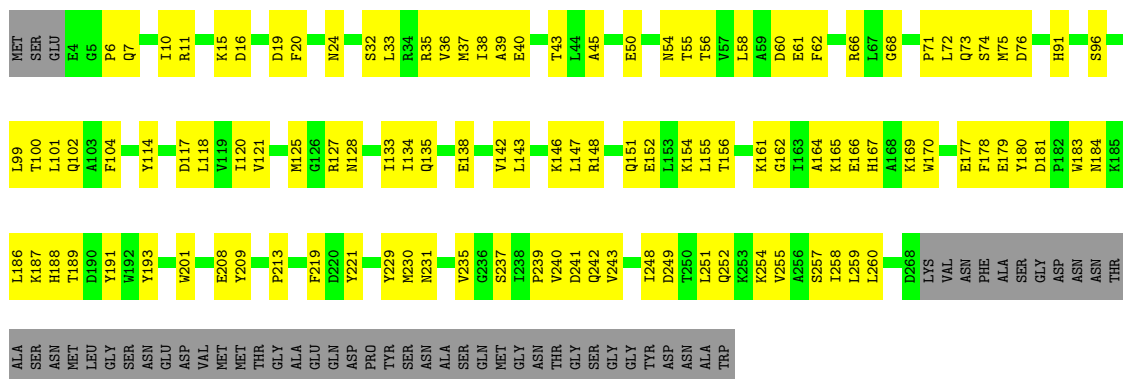


MET	SER	LEU	ALA	ASN	SER	GLU	LYS	TYR	TYR	PRO	ASP	GLU	ASP	E104	T109	TYR	GLY	PHE	GLU	D20	E21	S22	I25	D29	S35	L43	V44	L48	F51	N52	Y57	F58	L59	I62	S67	T68	L69	I70	E72	Q73	L74	A75	Q76	H77	T78	E79	S80	S81	D82	M83			
I84	S85	R86	K87	Y88	E89	I90	S91	P92	M101	Y102	ASP	ASP	E104	T109	TYR	GLY	PHE	GLU	D20	E21	S22	I25	D29	S35	L43	V44	L48	F51	N52	Y57	F58	L59	I62	S67	T68	L69	I70	E72	Q73	L74	A75	Q76	H77	T78	E79	S80	S81	D82	M83				
I172	M173	R174	R175	S176	K177	N178	L181	S182	E183	A184	T185	E104	T109	TYR	GLY	PHE	GLU	D20	E21	S22	I25	D29	S35	L43	V44	L48	F51	N52	Y57	F58	L59	I62	S67	T68	L69	I70	E72	Q73	L74	A75	Q76	H77	T78	E79	S80	S81	D82	M83					
G260	R261	GLY	S264	S265	R267	P274	Y275	I276	Q277	Q278	D279	E280	F281	I282	V283	I284	R287	D198	M199	G200	N121	N122	T123	Y124	S125	G207	S208	E209	K210	V211	L212	I213	A214	Q215	E216	R217	V223	L234	V237	I324	Q325	D326	R327	E328	T329	L331	I334	G335	R336	K337	G338	T339	A340
L341	G342	K344	K345	E346	A347	R348	I349	Q350	K353	D354	I355	E359	F360	I282	V283	I284	R287	D198	M199	G200	N121	N122	T123	Y124	S125	G207	S208	E209	K210	V211	L212	I213	A214	Q215	E216	R217	V223	L234	V237	I324	Q325	D326	R327	E328	T329	L331	I334	G335	R336	K337	G338	T339	A340
L341	G342	K344	K345	E346	A347	R348	I349	Q350	K353	D354	I355	E359	F360	I282	V283	I284	R287	D198	M199	G200	N121	N122	T123	Y124	S125	G207	S208	E209	K210	V211	L212	I213	A214	Q215	E216	R217	V223	L234	V237	I324	Q325	D326	R327	E328	T329	L331	I334	G335	R336	K337	G338	T339	A340
I428	Y431	R434	K345	E346	A347	R348	I349	Q350	K353	D354	I355	E359	F360	I282	V283	I284	R287	D198	M199	G200	N121	N122	T123	Y124	S125	G207	S208	E209	K210	V211	L212	I213	A214	Q215	E216	R217	V223	L234	V237	I324	Q325	D326	R327	E328	T329	L331	I334	G335	R336	K337	G338	T339	A340
E526	G530	A531	A532	C533	G534	K537	N538	M542	I545	S546	S547	H548	M552	I555	L558	M563	L566	Q573	V580	F581	V582	V585	H590	N591	N592	P593	R594	R595	L596	M597	E598	L603	R604	I609	M610	P611	E612	L613	S614	M615	L616	R617	R620	E678	D709	L710	M789						
L624	R625	I626	D629	G631	R632	L637	F638	V640	E641	D642	H648	K649	E650	L651	I658	M662	D668	GLY	PHE	GLU	ASP	VAL	E678	Y679	T680	S683	L684	L685	N686	E687	G688	L689	V690	Y692	I693	E696	M705	Q706	P707	L782	T783	N784	D788	L710	M789								
A713	GLU	ALA	ASN	GLU	ASN	ASP	LEU	ASP	ASP	P80	A726	K727	R728	I729	A730	VAL	SER	HIS	HIS	A735	T736	T737	I743	H744	P745	S746	M747	A752	A753	P757	F758	P759	D760	H761	N762	Q763	S764	P765	Q770	S771	A772	K775	Q776	A777	M778	L782	T783	N784	D788	L710	M789		
A793	N794	I795	L796	K865	K866	G867	M868	P802	L803	G804	T805	T806	R807	A808	M809	E810	Y811	F814	P818	Q821	N822	A823	I824	A828	C829	Y830	S831	N834	Q835	E836	M839	I840	M841	N842	Q843	S844	S845	I846	D847	R848	F851	R852	L854	F855	R856	R857	S858	Y859	M860	D861			
Q862	E863	K864	K865	K866	G867	M868	P802	L803	G804	T805	T806	R807	A808	M809	E810	Y811	F814	P818	Q821	N822	A823	I824	A828	C829	Y830	S831	N834	Q835	E836	M839	I840	M841	N842	Q843	S844	S845	I846	D847	R848	F851	R852	L854	F855	R856	R857	S858	Y859	M860	D861				
H932	D936	T939	P940	L941	R942	S943	T944	E945	V949	G1042	D1043	A1044	S1045	F1046	F1047	T1051	G960	L961	F962	P963	V964	K965	Q975	I976	R977	D978	K979	P980	R983	K887	G988	T989	I990	G991	I992	T993	Y994	R995	R996	E997	D998	M999	P1000	V1007	P1008	D1009	L1010	I1011	I1012				
M1013	P1018	L1027	L1031	S1032	K1033	A1036	L1037	E1041	G1042	D1043	A1044	S1045	F1046	F1047	T1051	G960	L961	F962	P963	V964	K965	Q975	I976	R977	D978	K979	P980	R983	K887	G988	T989	I990	G991	I992	T993	Y994	R995	R996	E997	D998	M999	P1000	V1007	P1008	D1009	L1010	I1011	I1012					



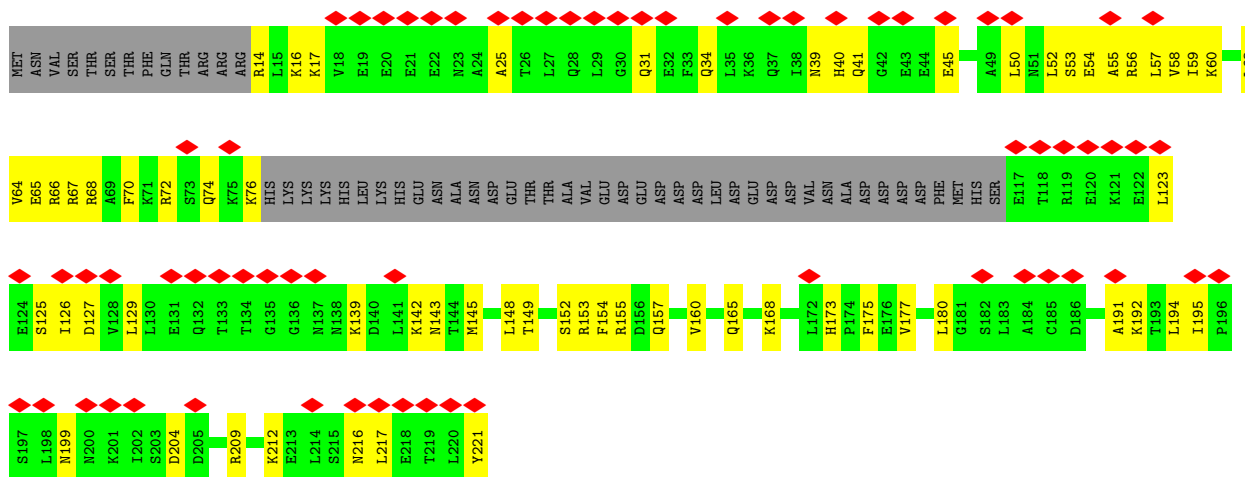
- Molecule 5: DNA-directed RNA polymerase II subunit RPB3

Chain C: 48% 35% 17%



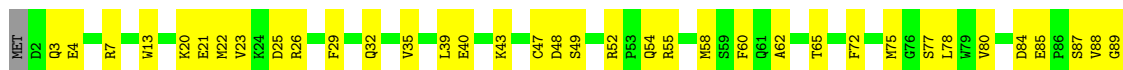
- Molecule 6: DNA-directed RNA polymerase II subunit RPB4

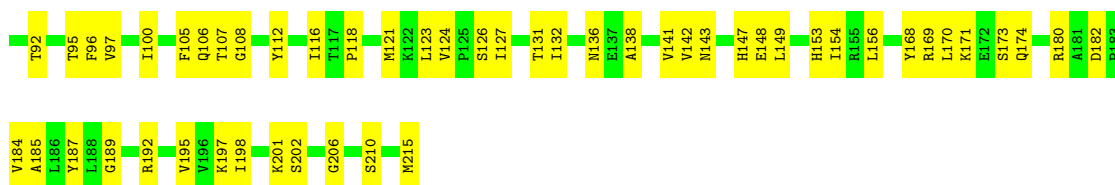
Chain D: 30% 47% 29% 24%



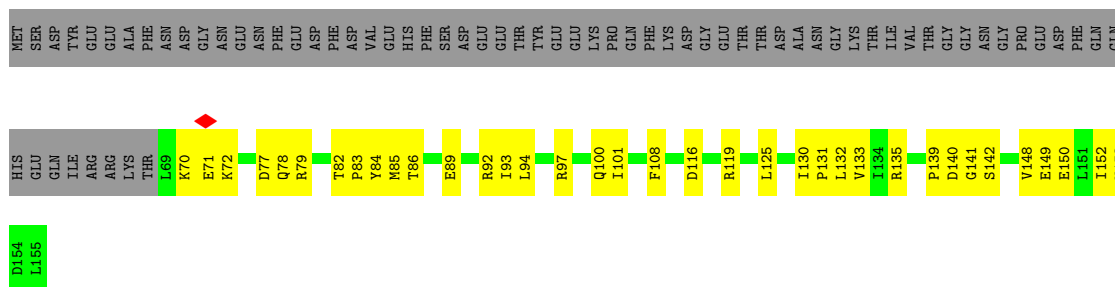
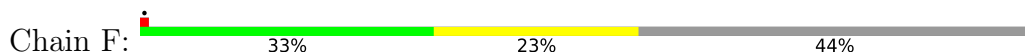
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPB3C1

Chain E: 59% 40%

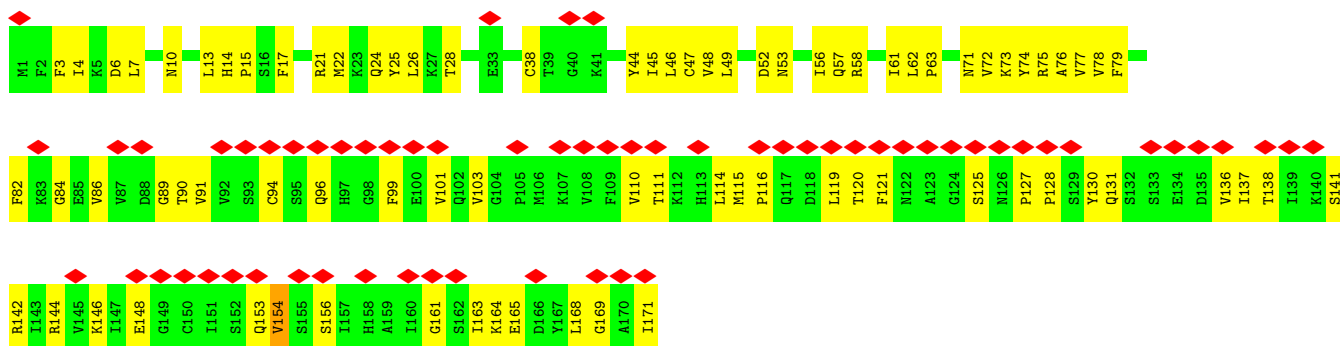




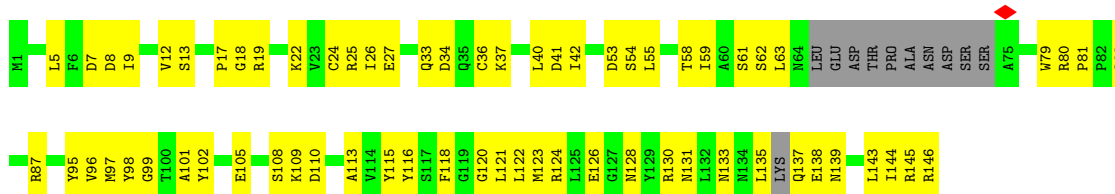
• Molecule 8: DNA-directed RNA polymerases I,II,and III subunit RPABC2



• Molecule 9: DNA-directed RNA polymerase II subunit RPB7

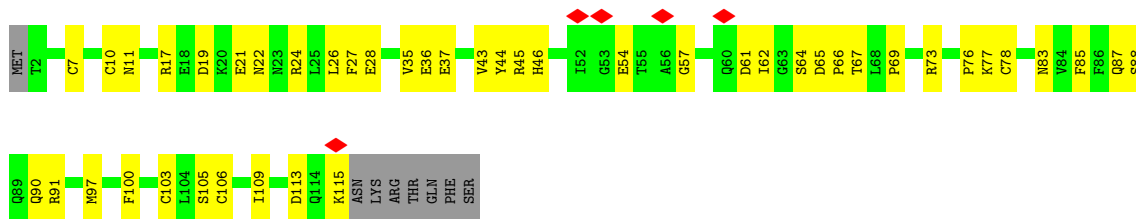


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC3

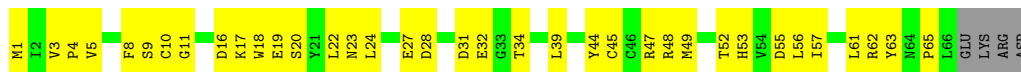


• Molecule 11: DNA-directed RNA polymerase II subunit RPB9

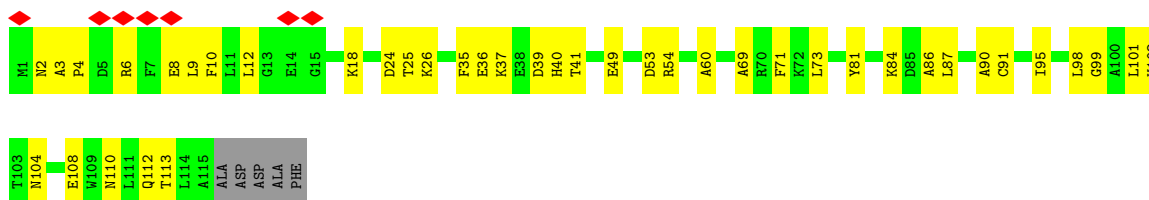




- Molecule 12: DNA-directed RNA polymerases II subunit RPABC5



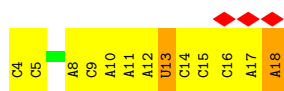
- Molecule 13: DNA-directed RNA polymerase II subunit RPB11



- Molecule 14: DNA-directed RNA polymerases II subunit RPABC4

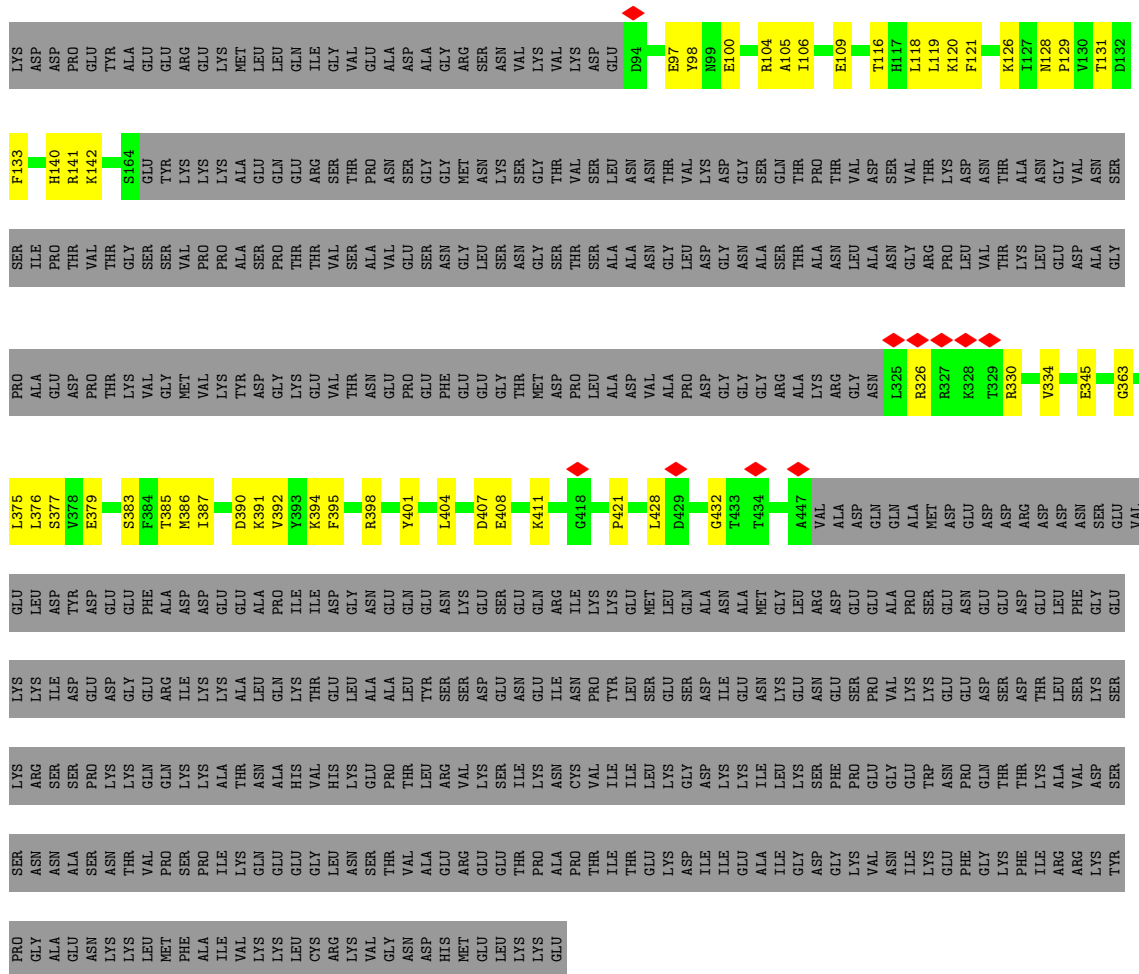


- Molecule 15: RNA (5'-R(P*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*CP*CP*CP*AP*A)-3')



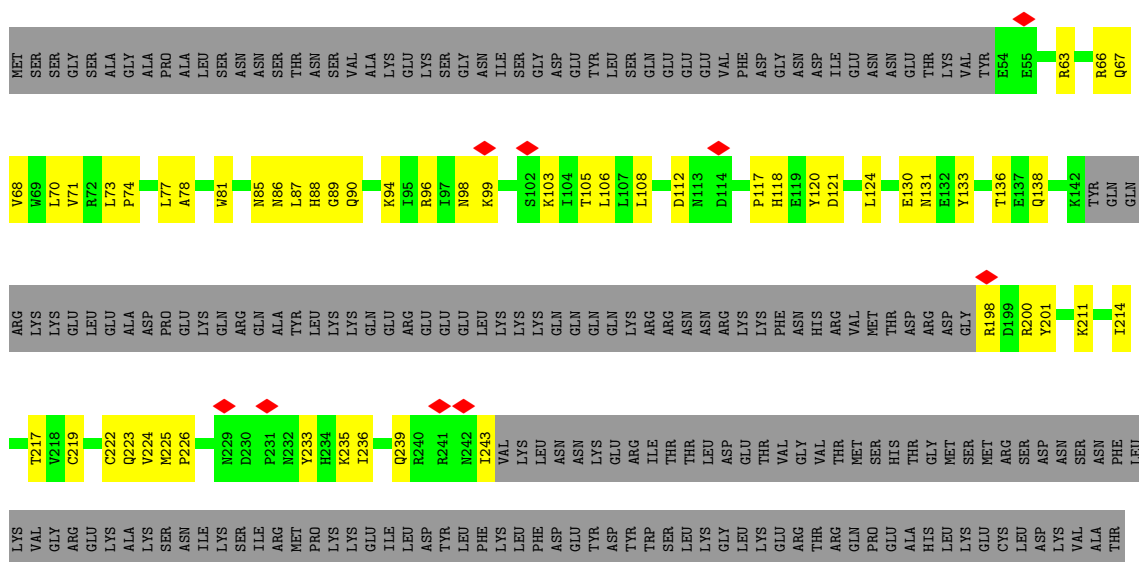
- Molecule 16: Transcription initiation factor IIF subunit alpha





● Molecule 17: Transcription initiation factor IIF subunit beta

Chain M: 20% 13% 66%



LEU VAL
LYS LYS
GLY PRO
TYR TYR
ALA PHE
LYS TYR
THR LEU
ARG PRO
GLU TYR
LYS LYS
LEU LYS
LYS GLU
GLU GLU
GLU ARG
LYS LYS
ALA THR
LEU LEU
GLY GLY
LEU LEU
ALA ASP
GLU GLN
THR GLY
SER SER
ALA GLY
GLY ASP
ASN ASP
ALA GLN
GLY ASP
ALA GLU
ALA ASP
LEU GLU
ASP ASP
GLU TLE
TLE GLU
MET MET
GLU ASP

VAL
VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	66261	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0084	Depositor
Map size (\AA)	237.6, 237.6, 237.6	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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	N	0.19	0/926	0.34	0/1425
2	O	0.28	0/925	0.53	0/1429
3	A	0.27	0/11368	0.49	2/15383 (0.0%)
4	B	0.28	0/9402	0.54	4/12680 (0.0%)
5	C	0.25	0/2124	0.44	0/2879
6	D	0.14	0/1339	0.39	0/1793
7	E	0.23	0/1788	0.42	0/2406
8	F	0.29	0/717	0.54	0/967
9	G	0.19	0/1363	0.48	0/1840
10	H	0.24	0/1097	0.47	0/1484
11	I	0.19	0/945	0.40	0/1273
12	J	0.36	0/549	0.59	0/738
13	K	0.25	0/942	0.44	0/1272
14	L	0.21	0/354	0.71	0/468
15	R	0.49	0/347	0.74	0/536
16	Q	0.17	0/1648	0.41	1/2226 (0.0%)
17	M	0.16	0/1124	0.43	0/1517
All	All	0.26	0/36958	0.49	7/50316 (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
3	A	0	3
4	B	0	3
9	G	0	1
All	All	0	7

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	421	PRO	N-CA-CB	7.66	110.16	103.27
4	B	79	THR	CA-C-N	6.46	133.32	121.70
4	B	79	THR	C-N-CA	6.46	133.32	121.70
4	B	918	ILE	CA-C-N	5.26	131.16	121.70
4	B	918	ILE	C-N-CA	5.26	131.16	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	252	PHE	Peptide
3	A	55	ASP	Peptide
3	A	750	GLY	Peptide
4	B	363	HIS	Peptide
4	B	510	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	N	822	0	449	19	0
2	O	827	0	458	19	0
3	A	11167	0	11188	485	0
4	B	9227	0	9200	418	0
5	C	2086	0	2045	98	0
6	D	1331	0	1344	57	0
7	E	1752	0	1776	70	0
8	F	705	0	731	33	0
9	G	1335	0	1346	58	0
10	H	1080	0	1049	61	0
11	I	927	0	881	37	0
12	J	540	0	553	37	0
13	K	924	0	934	42	0
14	L	352	0	375	20	0
15	R	312	0	165	12	0
16	Q	1619	0	1452	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	M	1106	0	1099	48	0
18	A	2	0	0	0	0
18	B	1	0	0	0	0
18	C	1	0	0	0	0
18	I	2	0	0	0	0
18	J	1	0	0	0	0
18	L	1	0	0	0	0
19	A	1	0	0	0	0
19	R	1	0	0	0	0
All	All	36122	0	35045	1403	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 20.

The worst 5 of 1403 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:510:LYS:HG3	4:B:511:PRO:HD3	1.45	0.98
12:J:8:PHE:H	12:J:49:MET:HE1	1.27	0.97
14:L:48:CYS:SG	14:L:51:CYS:HB2	2.09	0.93
3:A:110:CYS:HB3	3:A:167:CYS:SG	2.09	0.92
3:A:802:ASN:HD21	3:A:806:ARG:HB2	1.35	0.91

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	1417/1733 (82%)	1266 (89%)	148 (10%)	3 (0%)	43	73
4	B	1150/1224 (94%)	1001 (87%)	147 (13%)	2 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	263/318 (83%)	231 (88%)	32 (12%)	0	100	100
6	D	164/221 (74%)	159 (97%)	5 (3%)	0	100	100
7	E	212/215 (99%)	196 (92%)	16 (8%)	0	100	100
8	F	85/155 (55%)	77 (91%)	8 (9%)	0	100	100
9	G	169/171 (99%)	155 (92%)	14 (8%)	0	100	100
10	H	129/146 (88%)	110 (85%)	19 (15%)	0	100	100
11	I	112/122 (92%)	102 (91%)	10 (9%)	0	100	100
12	J	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
13	K	113/120 (94%)	108 (96%)	5 (4%)	0	100	100
14	L	42/70 (60%)	30 (71%)	12 (29%)	0	100	100
16	Q	208/735 (28%)	202 (97%)	6 (3%)	0	100	100
17	M	131/400 (33%)	123 (94%)	8 (6%)	0	100	100
All	All	4259/5700 (75%)	3814 (90%)	440 (10%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	188	ASP
4	B	364	ILE
3	A	195	ASP
3	A	253	ASN
4	B	363	HIS

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	
3	A	1235/1520 (81%)	1231 (100%)	4 (0%)	86	83
4	B	1000/1061 (94%)	997 (100%)	3 (0%)	86	83
5	C	233/274 (85%)	233 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	D	146/200 (73%)	146 (100%)	0	100	100
7	E	196/197 (100%)	196 (100%)	0	100	100
8	F	77/137 (56%)	77 (100%)	0	100	100
9	G	151/152 (99%)	151 (100%)	0	100	100
10	H	118/128 (92%)	118 (100%)	0	100	100
11	I	108/116 (93%)	108 (100%)	0	100	100
12	J	61/65 (94%)	61 (100%)	0	100	100
13	K	99/102 (97%)	99 (100%)	0	100	100
14	L	39/57 (68%)	39 (100%)	0	100	100
16	Q	147/641 (23%)	147 (100%)	0	100	100
17	M	125/363 (34%)	125 (100%)	0	100	100
All	All	3735/5013 (74%)	3728 (100%)	7 (0%)	85	85

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	195	ASP
4	B	264	SER
4	B	1183	LYS
4	B	265	SER
3	A	193	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
6	D	150	ASN
11	I	87	GLN
7	E	114	ASN
9	G	117	GLN
13	K	40	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	14/15 (93%)	8 (57%)	0

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	5	C
15	R	8	A
15	R	9	C
15	R	10	A
15	R	11	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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.

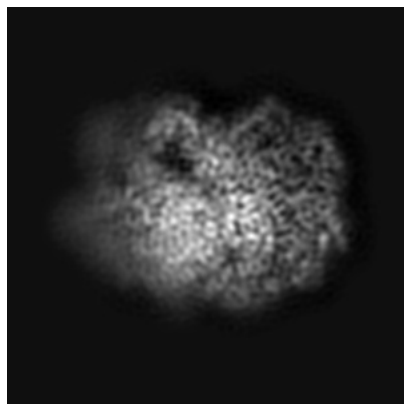
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23887. These allow visual inspection of the internal detail of the map and identification of artifacts.

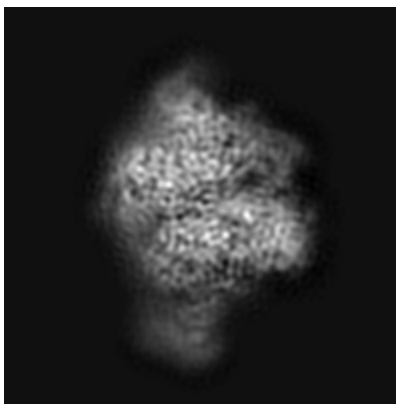
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

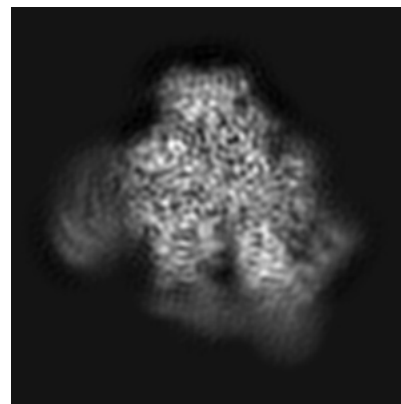
6.1.1 Primary map



X

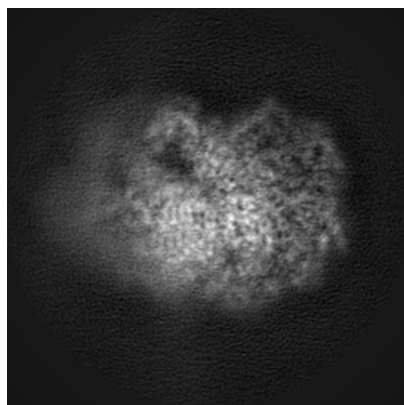


Y

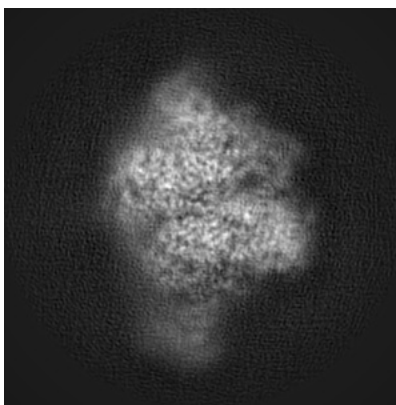


Z

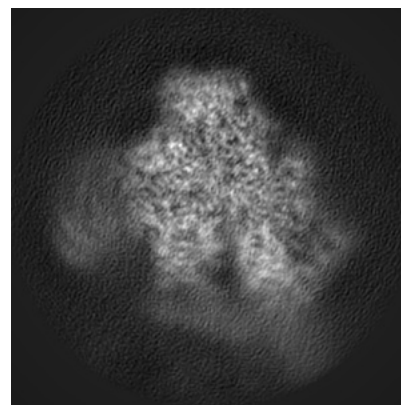
6.1.2 Raw map



X



Y

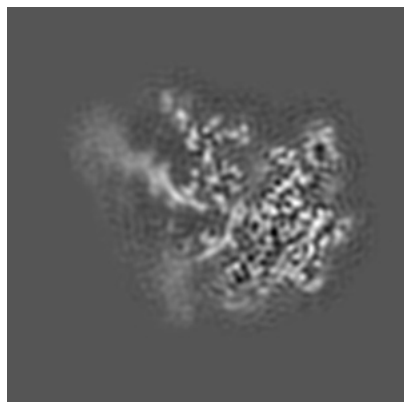


Z

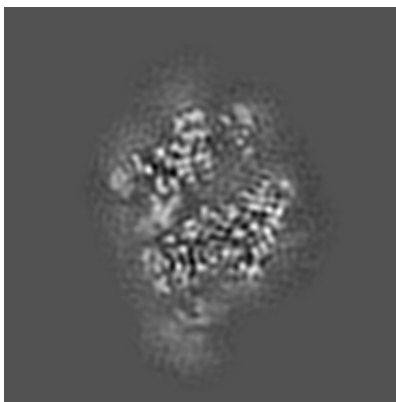
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

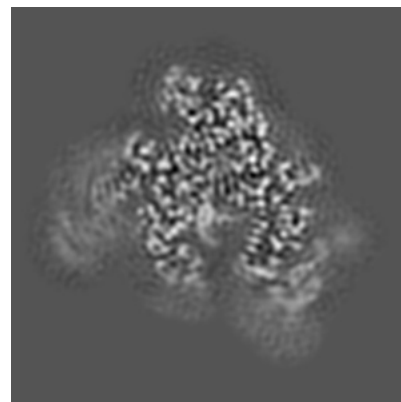
6.2.1 Primary map



X Index: 110

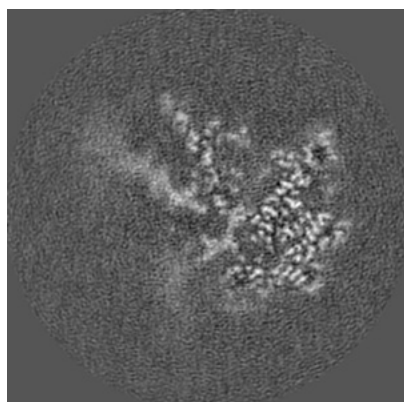


Y Index: 110

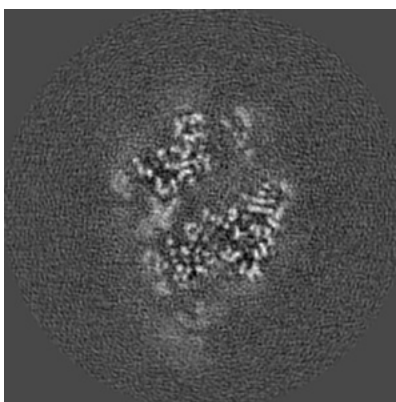


Z Index: 110

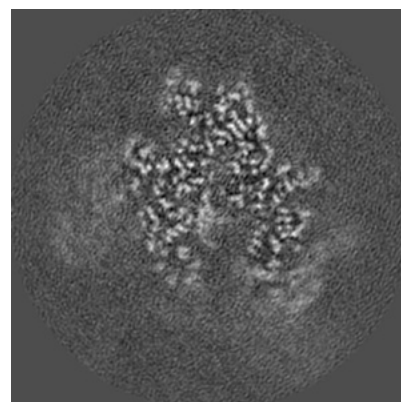
6.2.2 Raw map



X Index: 110



Y Index: 110

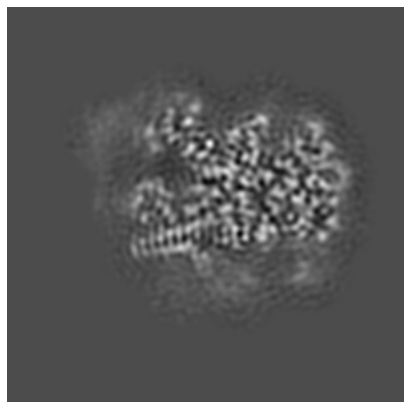


Z Index: 110

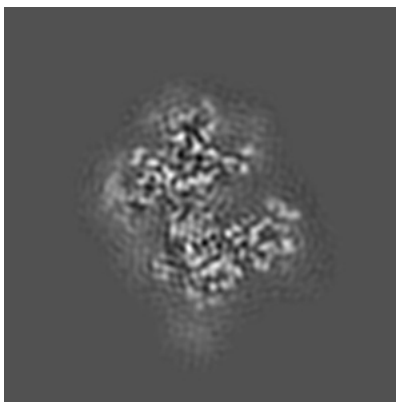
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

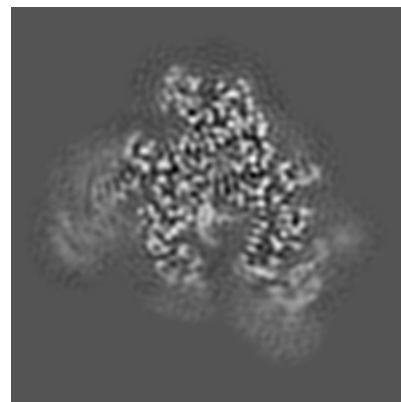
6.3.1 Primary map



X Index: 96

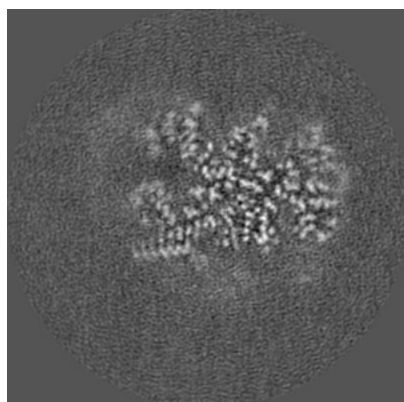


Y Index: 131

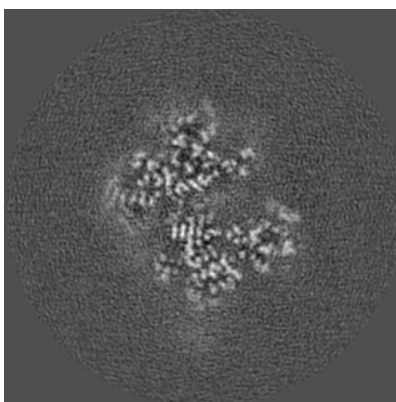


Z Index: 110

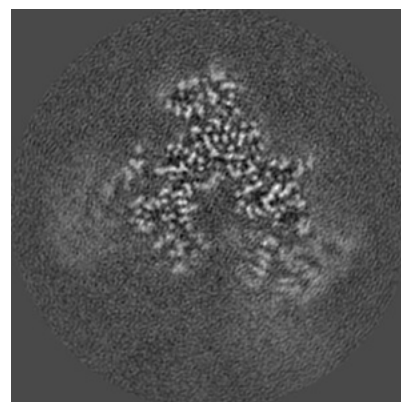
6.3.2 Raw map



X Index: 95



Y Index: 131

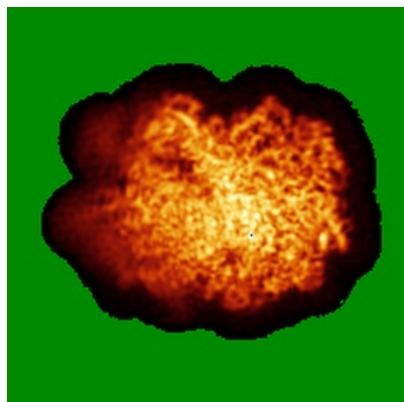


Z Index: 101

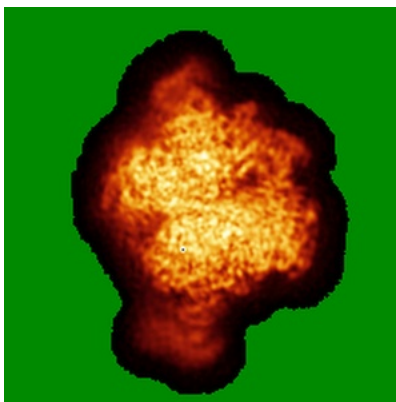
The images above show the largest variance slices of the map in three orthogonal directions.

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

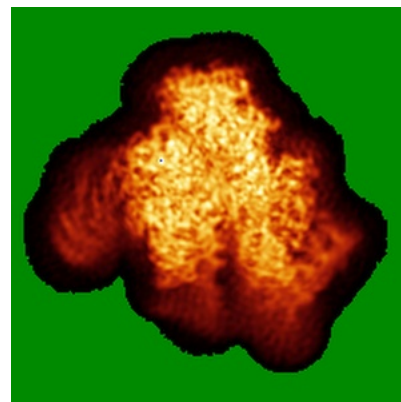
6.4.1 Primary map



X

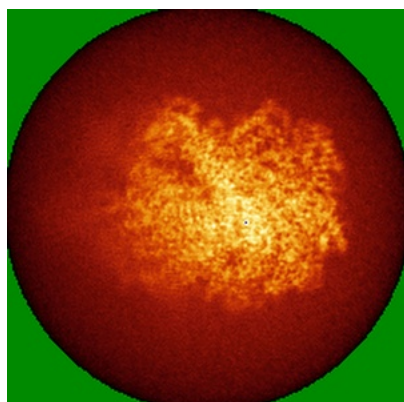


Y

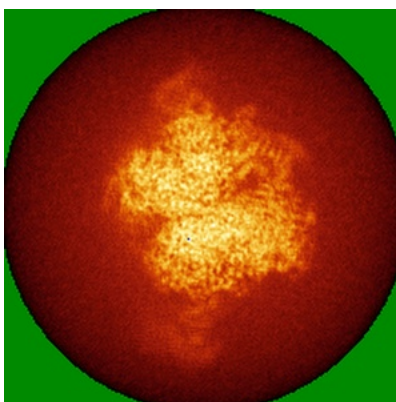


Z

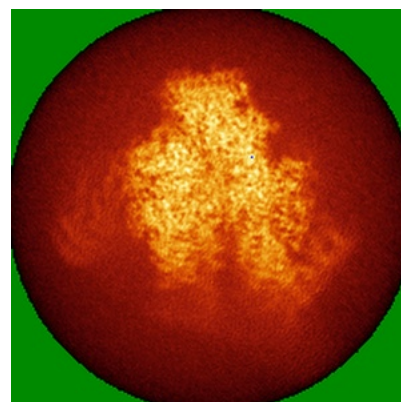
6.4.2 Raw map



X



Y

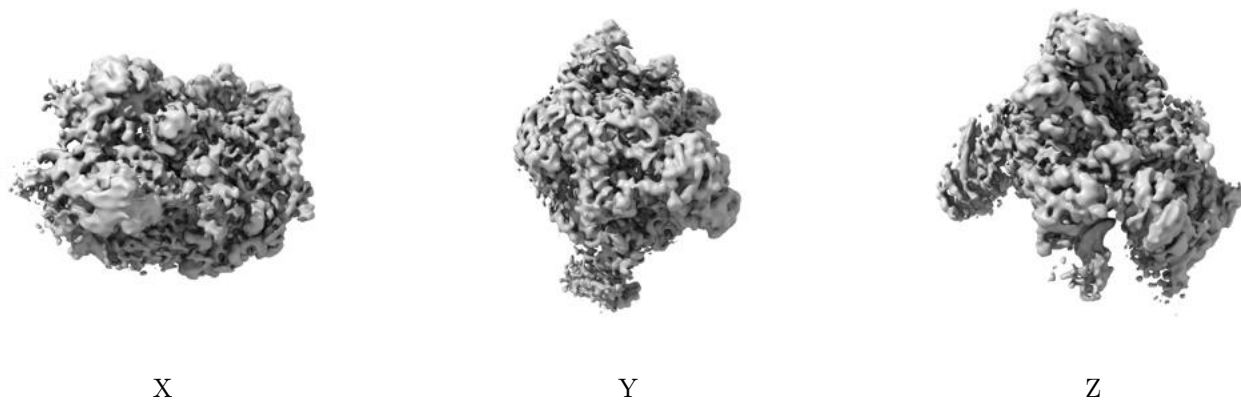


Z

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.

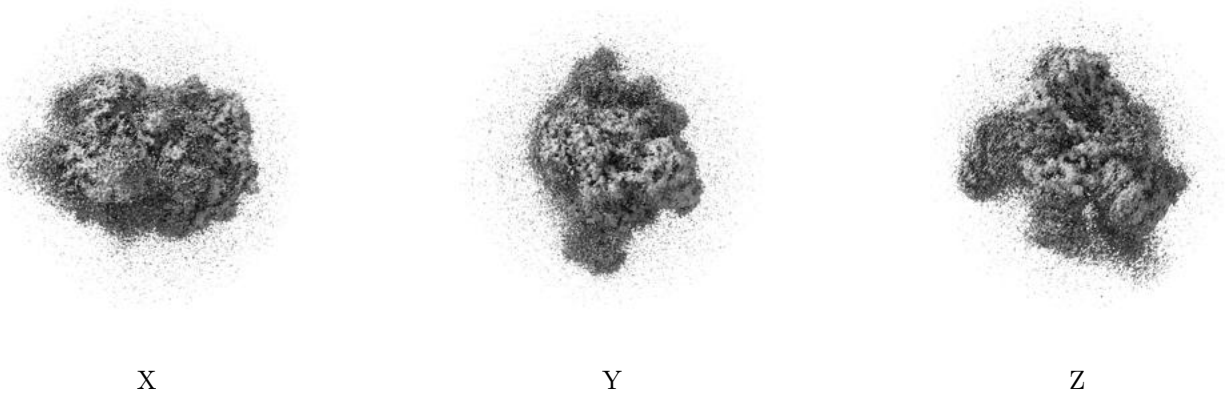
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0084. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

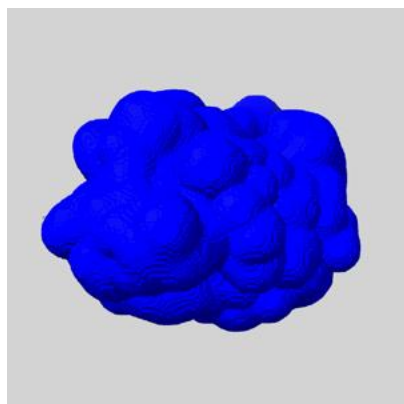
6.6 Mask visualisation [i](#)

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

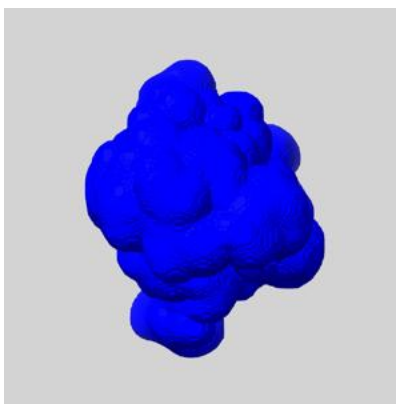
A mask typically either:

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

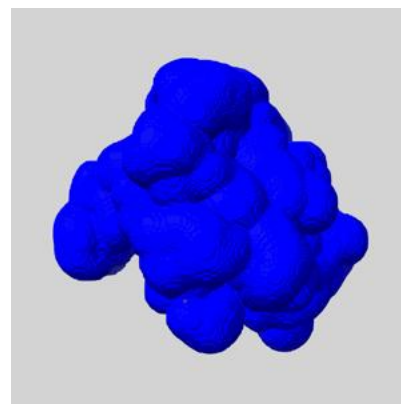
6.6.1 emd_23887_msk_1.map [i](#)



X



Y

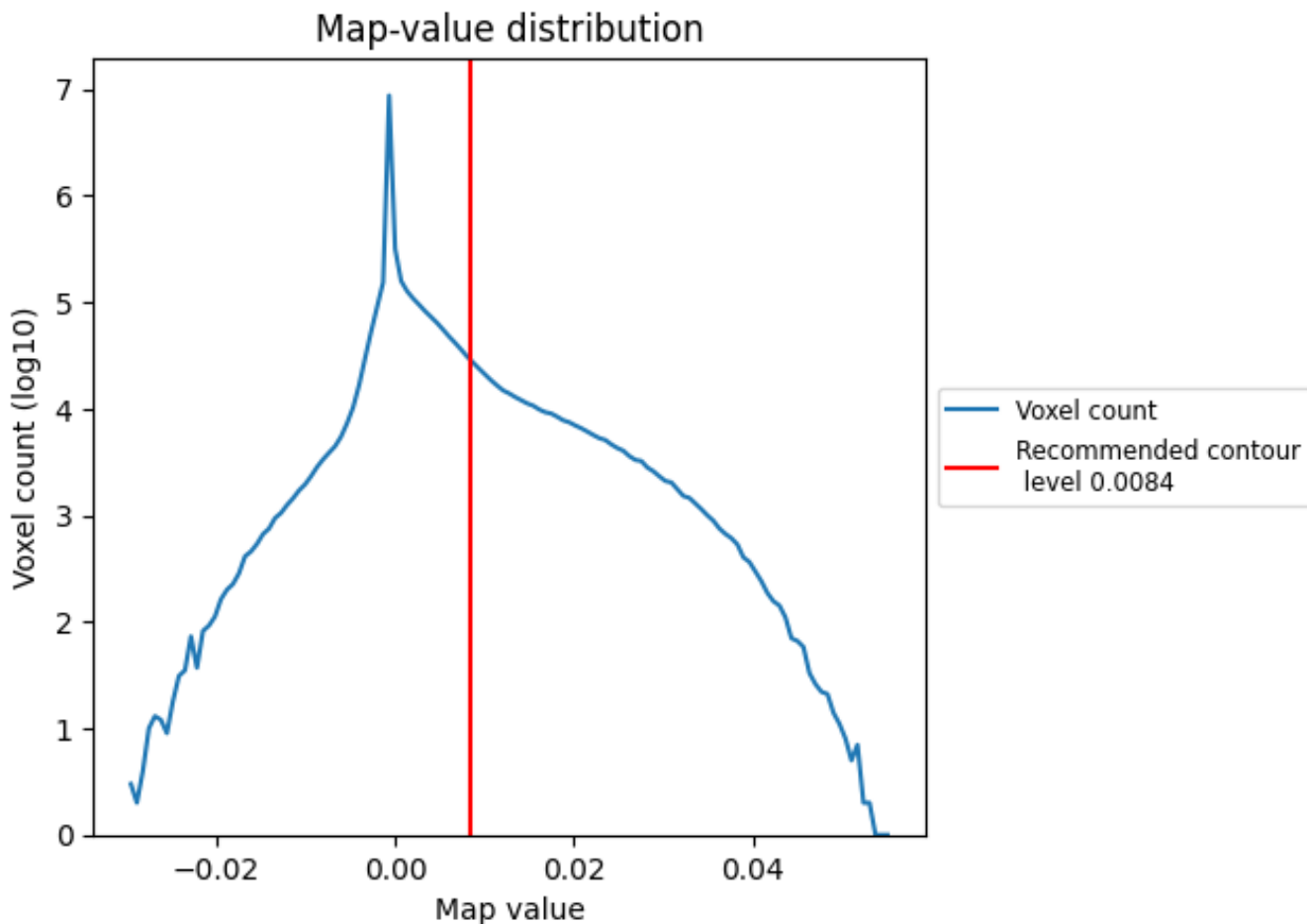


Z

7 Map analysis [i](#)

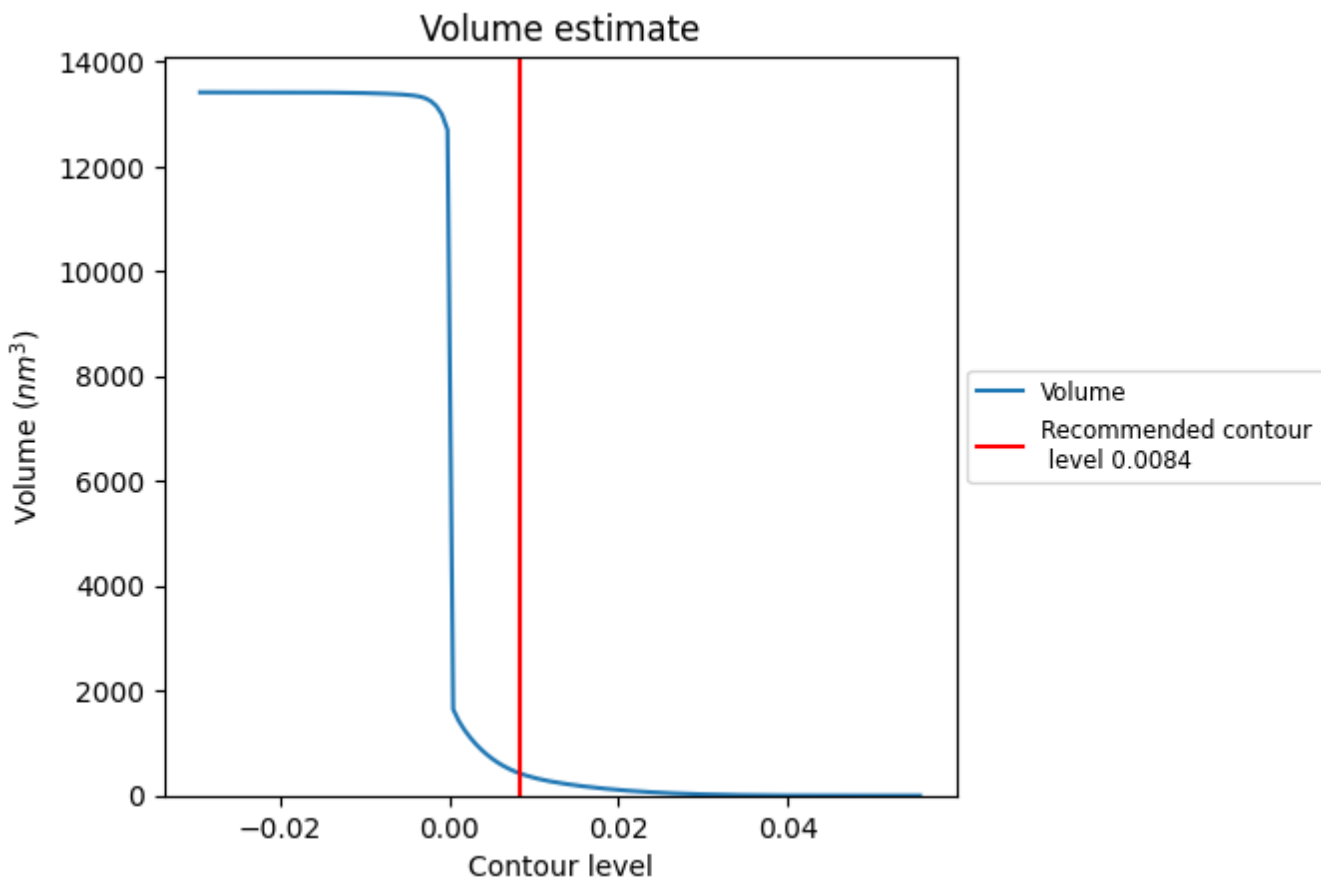
This section contains the results of statistical analysis of the map.

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.

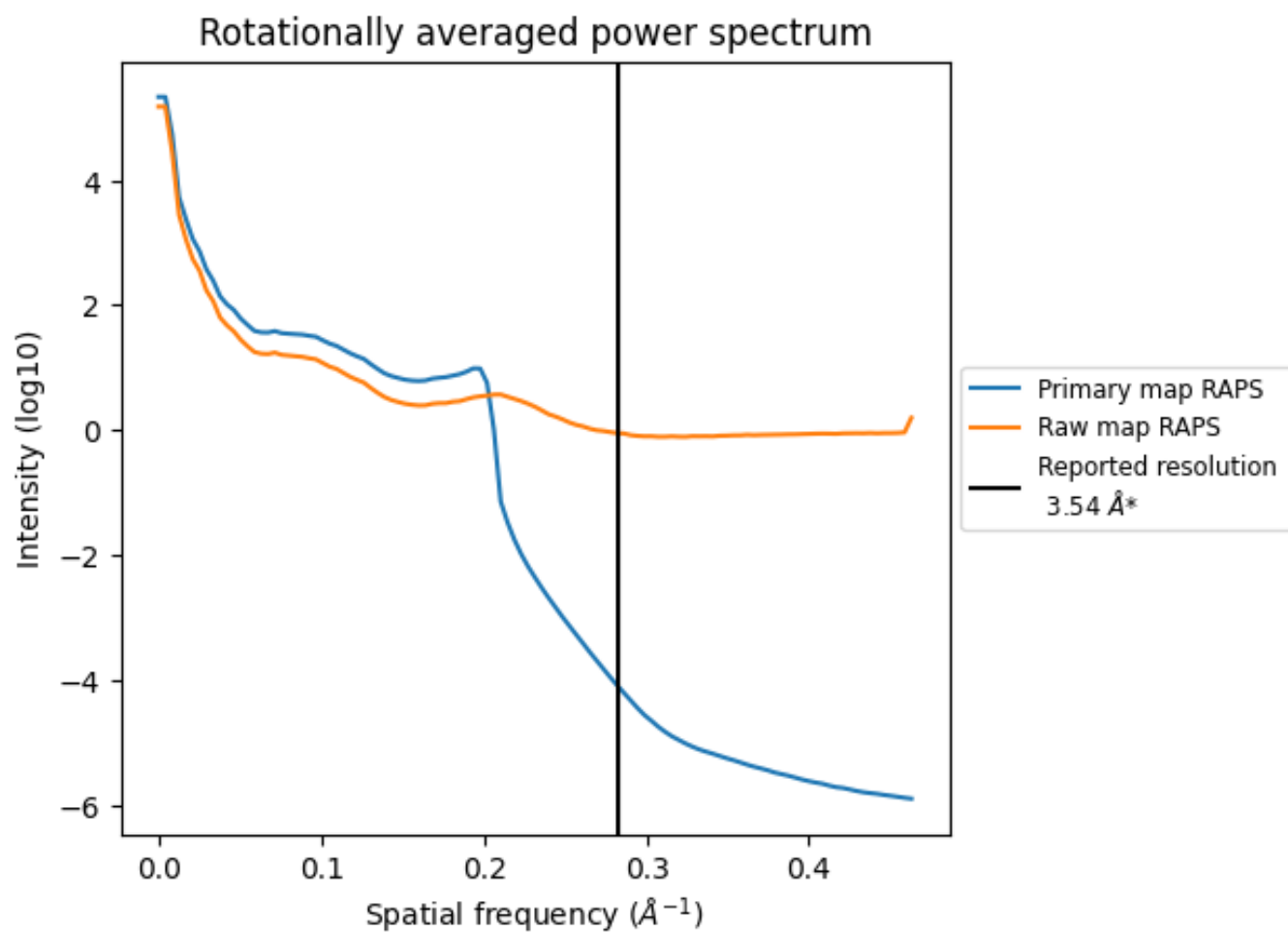
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 420 nm³; this corresponds to an approximate mass of 379 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](#)

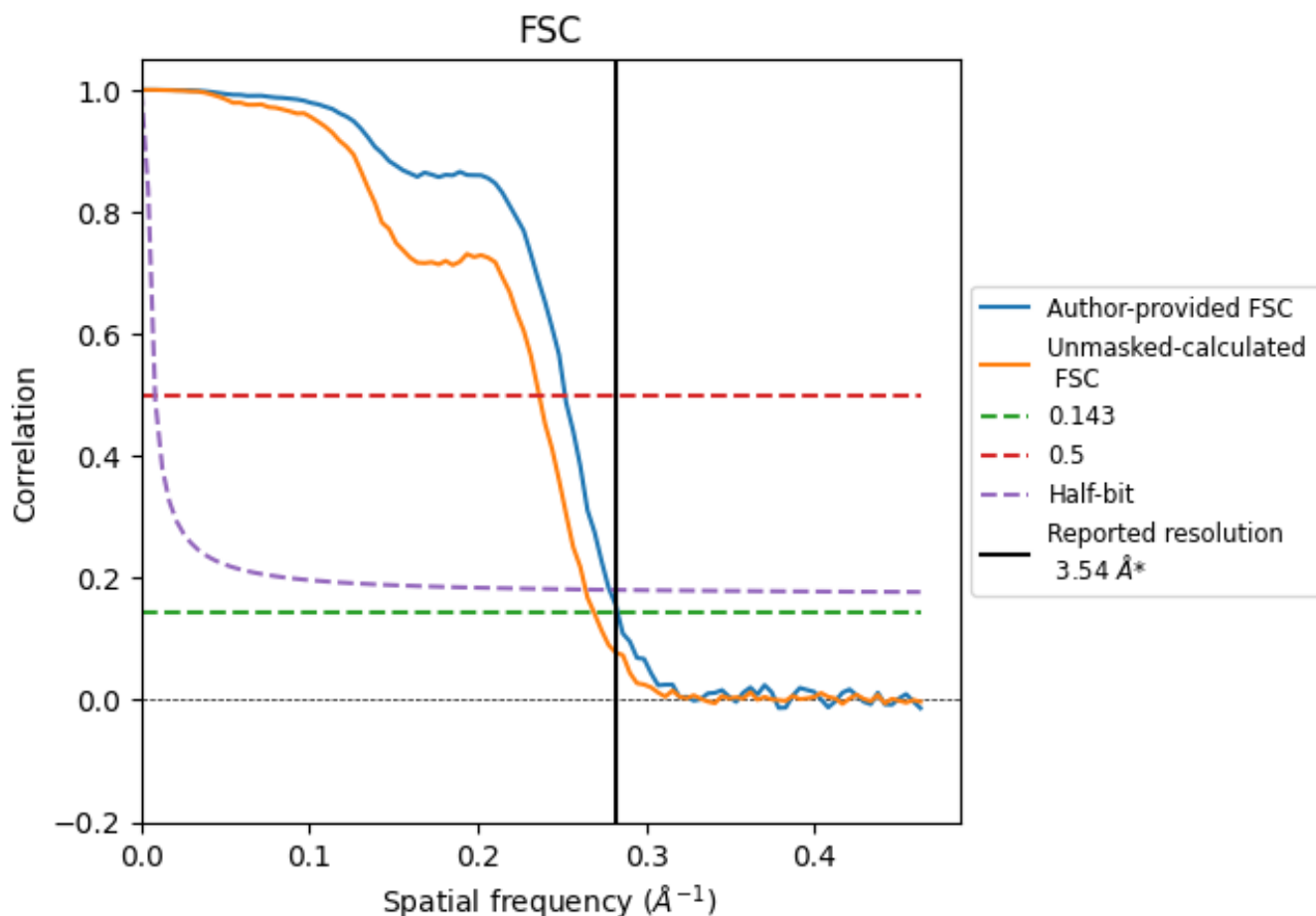


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

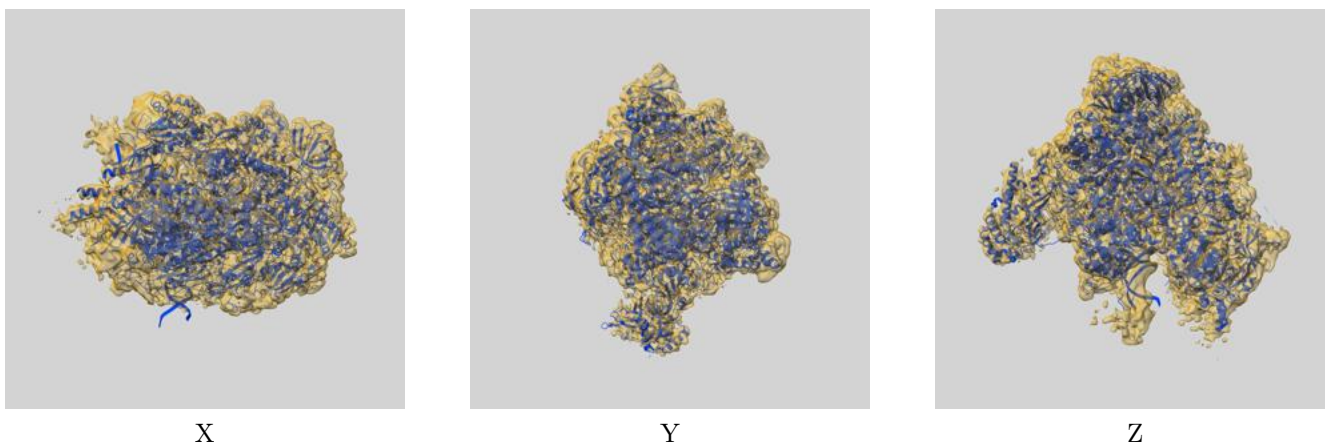
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	3.53	3.97	3.59
Unmasked-calculated*	3.72	4.23	3.79

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

9 Map-model fit [i](#)

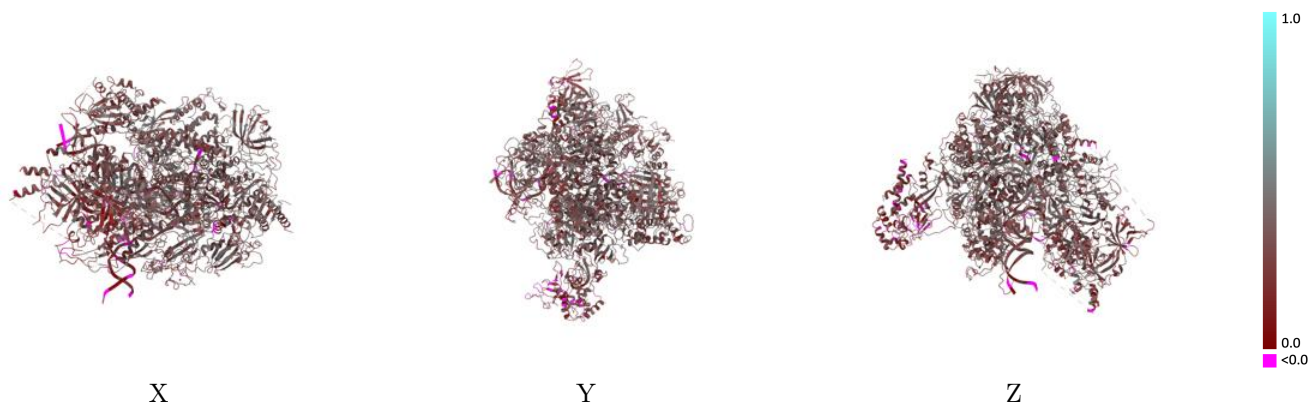
This section contains information regarding the fit between EMDB map EMD-23887 and PDB model 7MK9. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



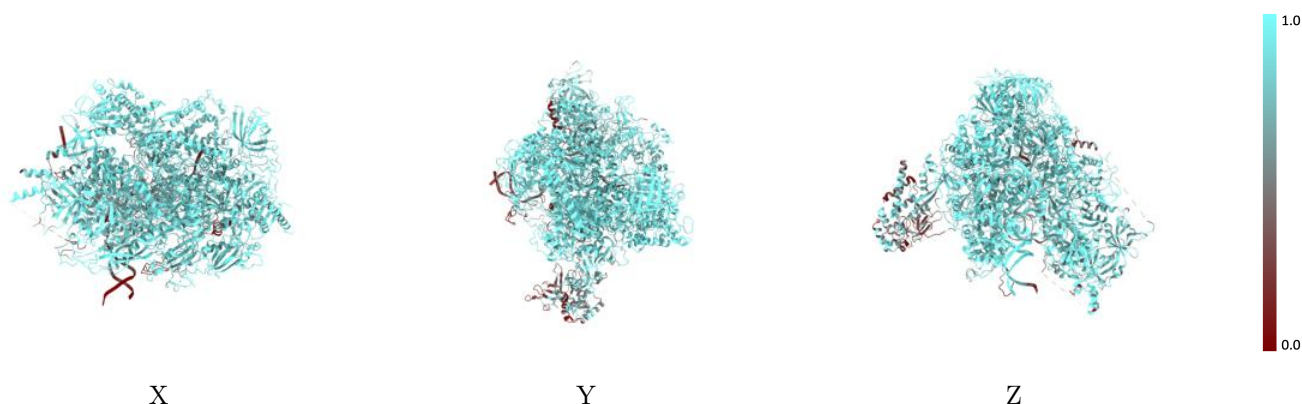
The images above show the 3D surface view of the map at the recommended contour level 0.0084 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



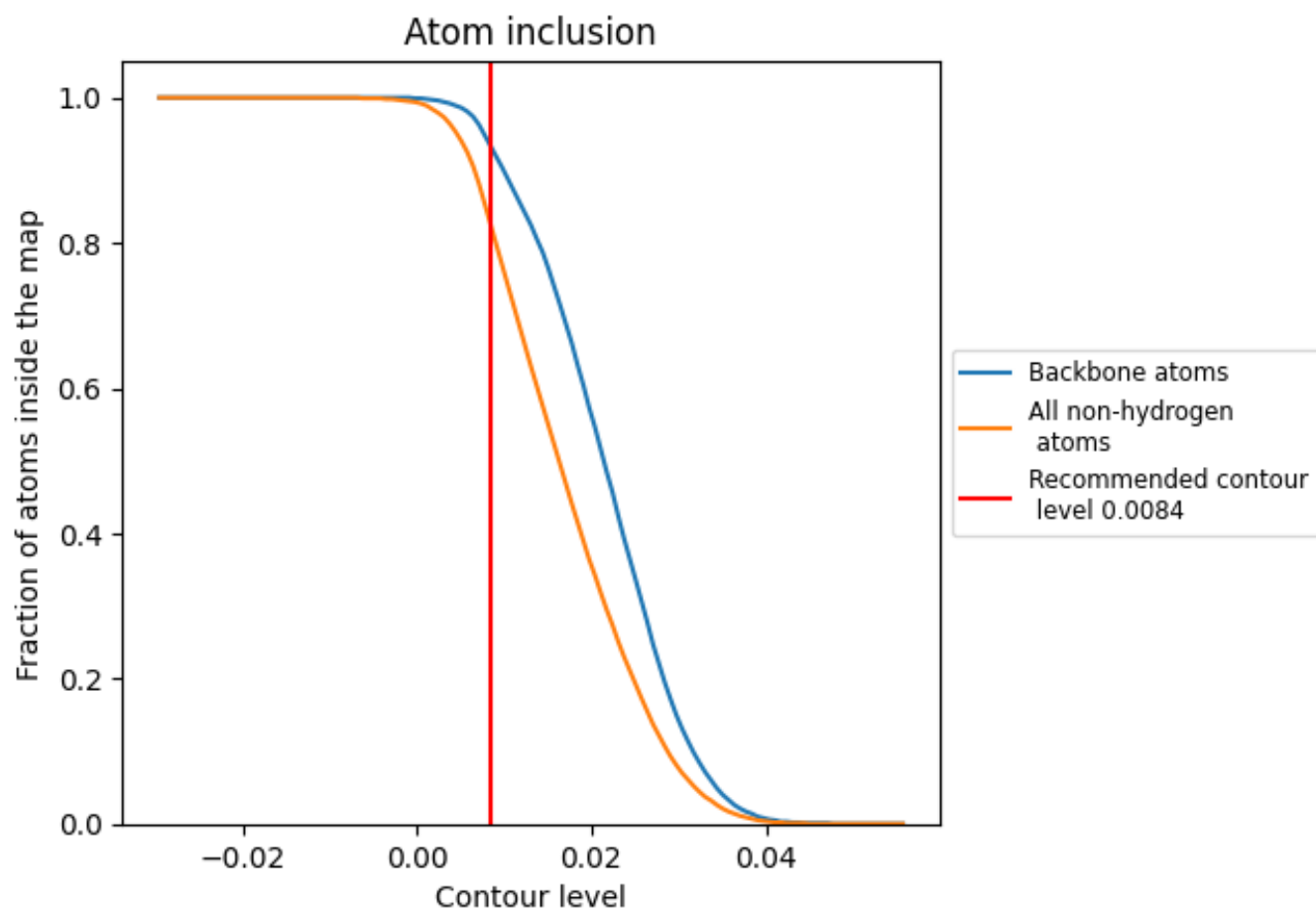
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0084).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 83% 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 (0.0084) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8270	 0.3170
A	 0.8810	 0.3470
B	 0.8380	 0.3360
C	 0.9000	 0.3600
D	 0.5130	 0.1930
E	 0.9050	 0.3440
F	 0.8750	 0.3580
G	 0.5470	 0.1910
H	 0.9300	 0.3400
I	 0.8800	 0.3390
J	 0.9290	 0.3570
K	 0.8330	 0.3200
L	 0.9000	 0.3260
M	 0.7830	 0.2340
N	 0.5910	 0.1750
O	 0.7400	 0.2100
Q	 0.7520	 0.2700
R	 0.7440	 0.2300

