



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:12 AM UTC

PDB ID : 8J90 / pdb_00008j90
EMDB ID : EMD-36083
Title : Cryo-EM structure of DDM1-nucleosome complex
Authors : Osakabe, A.; Takizawa, Y.; Horikoshi, N.; Hatazawa, S.; Berger, F.; Kurumizaka, H.; Kakutani, T.
Deposited on : 2023-05-02
Resolution : 4.71 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

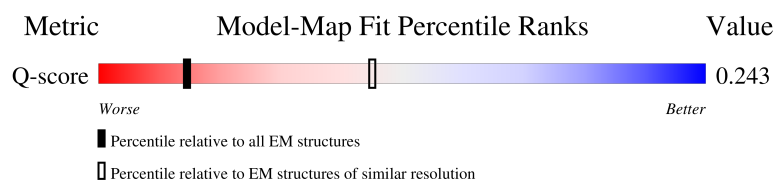
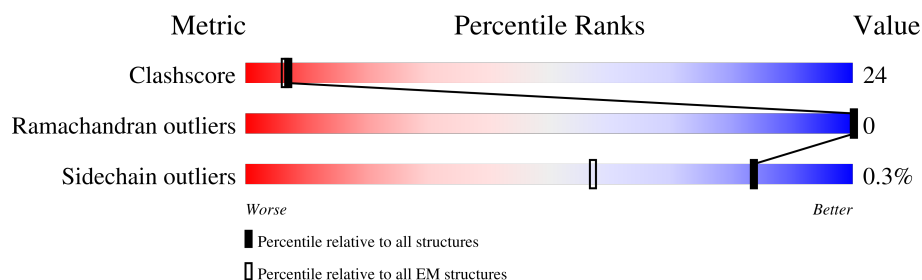
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

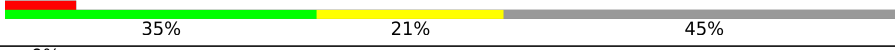
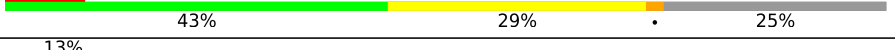
The reported resolution of this entry is 4.71 Å.

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	1656 (4.21 - 5.20)

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	139	
1	E	139	
2	B	106	
2	F	106	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	153	
3	G	153	
4	D	153	
4	H	153	
5	I	169	
6	J	169	
7	K	767	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13881 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 Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	74	Total	C	N	O	S	0	0
			598	379	113	104	2		
1	E	77	Total	C	N	O	S	0	0
			621	393	116	110	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P59226
A	-2	SER	-	expression tag	UNP P59226
A	-1	HIS	-	expression tag	UNP P59226
E	-3	GLY	-	expression tag	UNP P59226
E	-2	SER	-	expression tag	UNP P59226
E	-1	HIS	-	expression tag	UNP P59226

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	79	Total	C	N	O	S	0	0
			636	400	126	109	1		
2	F	84	Total	C	N	O	S	0	0
			676	425	135	115	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P59259
B	-2	SER	-	expression tag	UNP P59259
B	-1	HIS	-	expression tag	UNP P59259
F	-3	GLY	-	expression tag	UNP P59259
F	-2	SER	-	expression tag	UNP P59259
F	-1	HIS	-	expression tag	UNP P59259

- Molecule 3 is a protein called HTA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	88	Total	C	N	O	S	0	0
			676	431	128	115	2		
3	G	82	Total	C	N	O	S	0	0
			635	406	120	108	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q9FJE8
C	-2	SER	-	expression tag	UNP Q9FJE8
C	-1	HIS	-	expression tag	UNP Q9FJE8
G	-3	GLY	-	expression tag	UNP Q9FJE8
G	-2	SER	-	expression tag	UNP Q9FJE8
G	-1	HIS	-	expression tag	UNP Q9FJE8

- Molecule 4 is a protein called HTB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	90	Total	C	N	O	S	0	0
			703	451	119	131	2		
4	H	90	Total	C	N	O	S	0	0
			703	451	119	131	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP O23629
D	-2	SER	-	expression tag	UNP O23629
D	-1	HIS	-	expression tag	UNP O23629
H	-3	GLY	-	expression tag	UNP O23629
H	-2	SER	-	expression tag	UNP O23629
H	-1	HIS	-	expression tag	UNP O23629

- Molecule 5 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	111	Total	C	N	O	P	0	0
			2260	1072	410	667	111		

- Molecule 6 is a DNA chain called DNA (169-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	111	Total	C	N	O	P	0	0
			2291	1082	433	665	111		

- Molecule 7 is a protein called ATP-dependent DNA helicase DDM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	504	Total	C	N	O	S	0	0
			4082	2603	724	735	20		

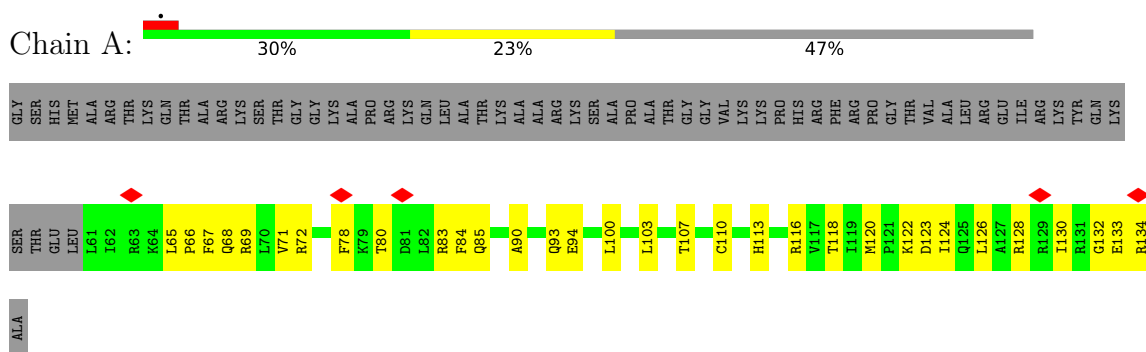
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-2	GLY	-	expression tag	UNP Q9XFH4
K	-1	PRO	-	expression tag	UNP Q9XFH4
K	0	HIS	-	expression tag	UNP Q9XFH4

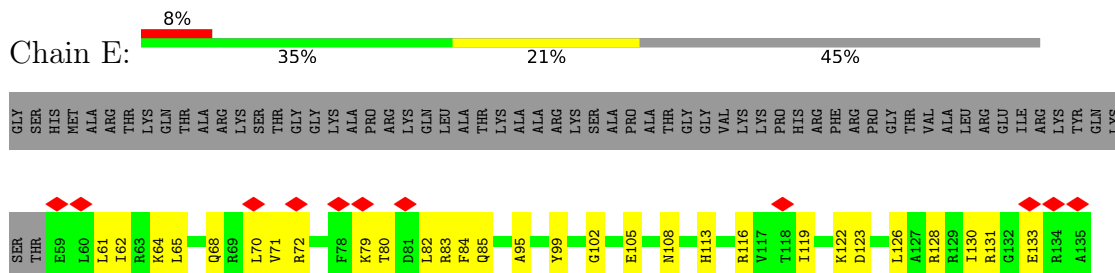
3 Residue-property plots [i](#)

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.

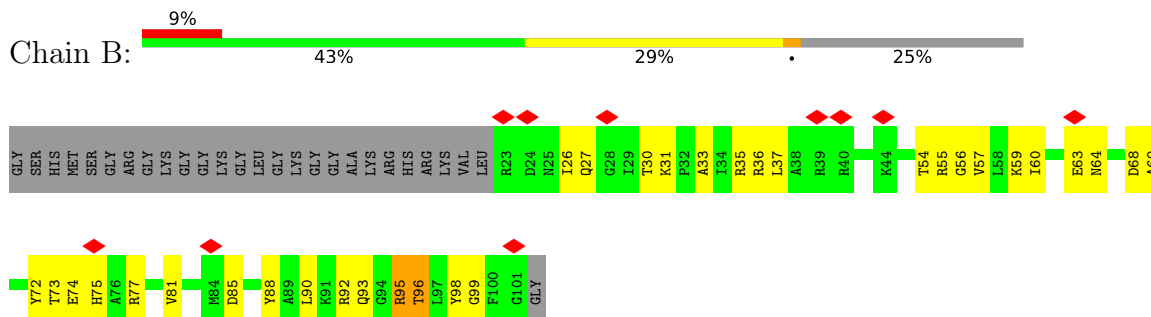
• Molecule 1: Histone H3.1



• Molecule 1: Histone H3.1

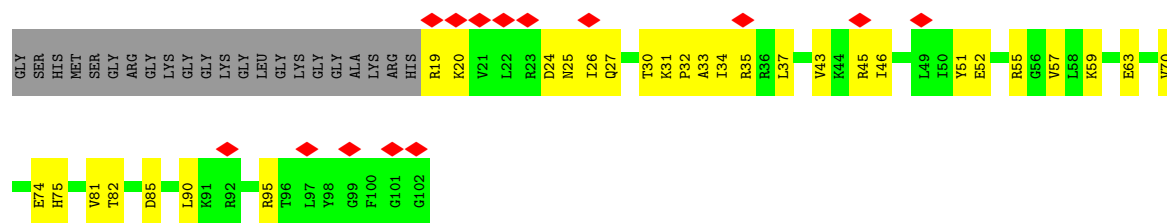


• Molecule 2: Histone H4

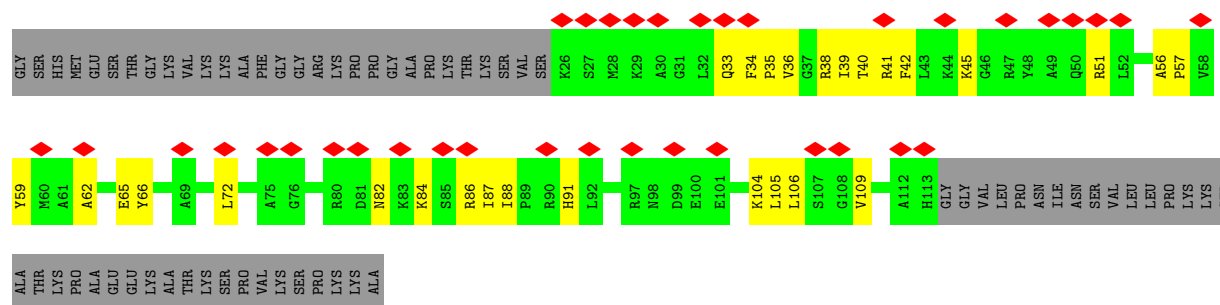
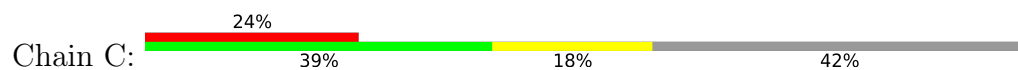


• Molecule 2: Histone H4

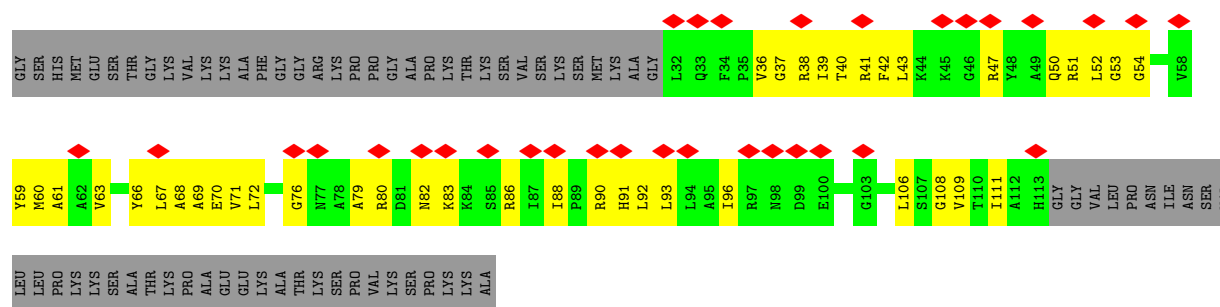
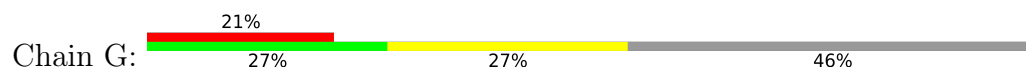




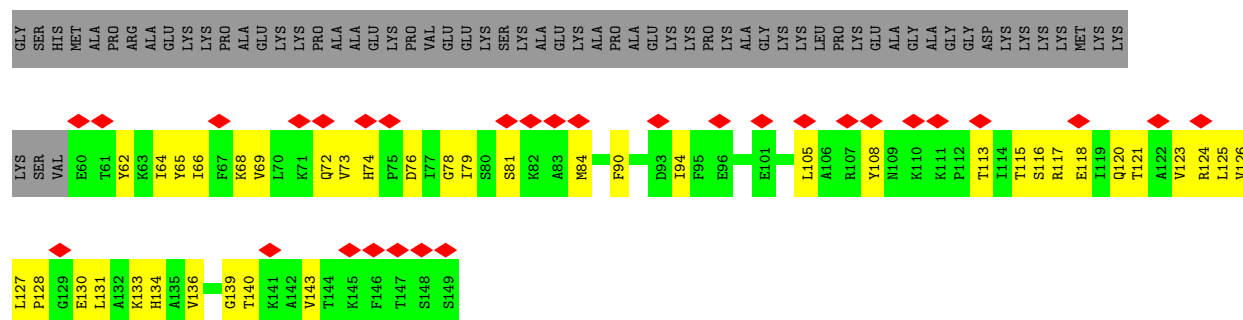
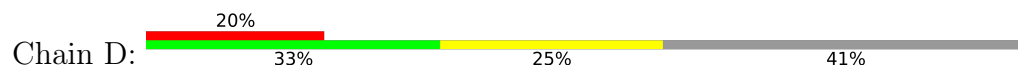
• Molecule 3: HTA6



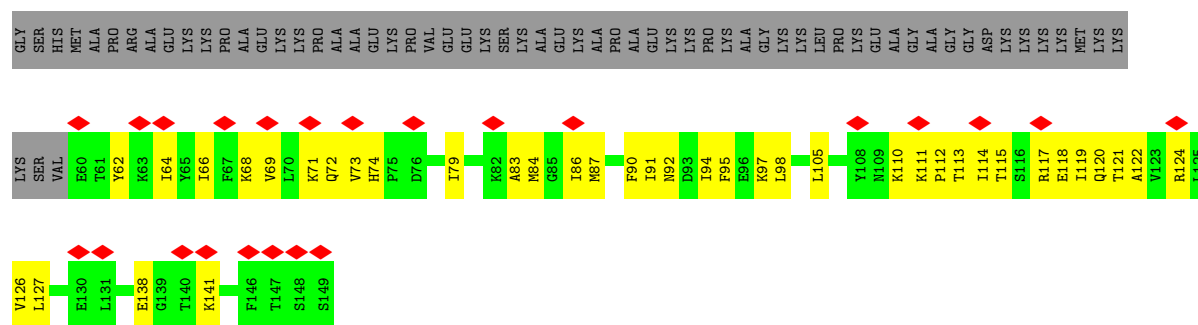
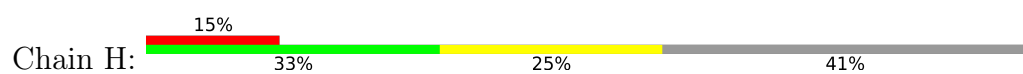
• Molecule 3: HTA6



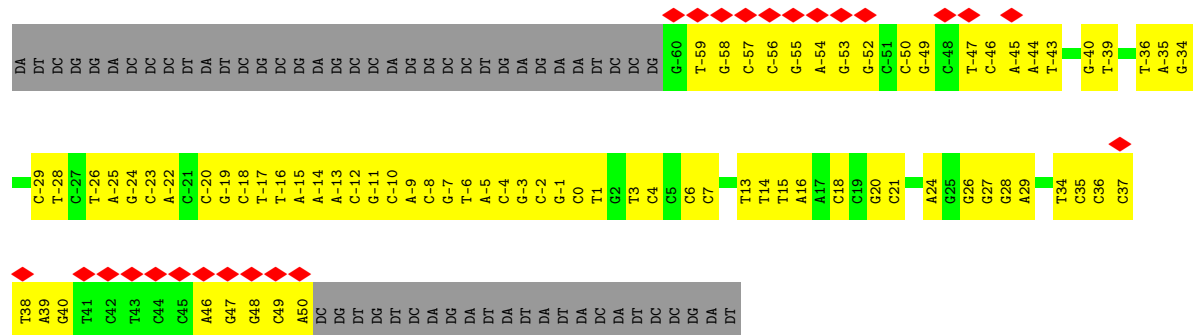
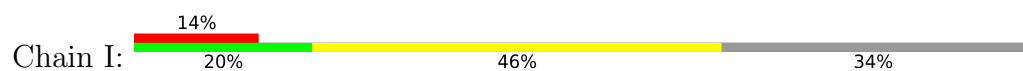
• Molecule 4: HTB9



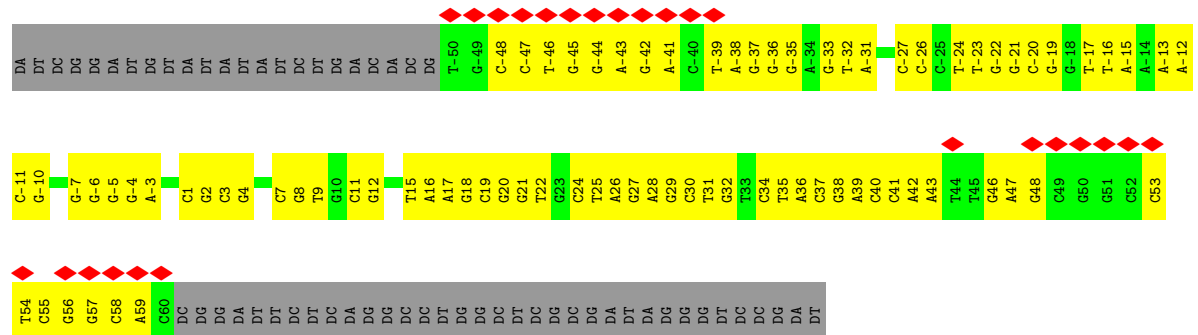
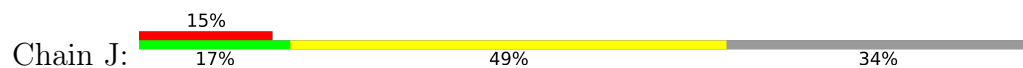
• Molecule 4: HTB9



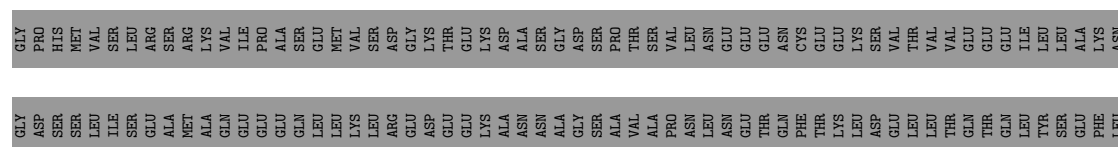
• Molecule 5: DNA (169-MER)



• Molecule 6: DNA (169-MER)



• Molecule 7: ATP-dependent DNA helicase DDM1



ASP	LEU	THR	ILE	THR	ALA	PRO	GLY	THR	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
A602	G603	G604	L605	G606	I607	Q608	L609	T610	A611	A612	D613	T614	C615	C616	L617	V618	D619	S620	D621	W622	N623	P624	Q625	M626	D627	L628	Q629	A630	I631	D632	G633	C634	H635	R636	I637	G638	Q639	T640	K641	P642	V643	H644	V645	Y646	D647	L648	S649	T650	A651	Q652	S653	I654	E655	T656	R657	R661	A662	Y663
K542	V543	L544	I545	F546	S547	Q548	T550	K551	L552	L553	D554	I555	M556	D557	Y558	Y559	F560	S561	E562	K563	G564	F565	E566	V567	C568	R569	I570	D571	G572	S573	V574	K575	L576	D577	E578	R579	R580	R581	Q582	I583	K584	D585	F586	S587	D588	E589	K590	S591	S592	C593	S594	I595	F596	L597	L598	S599	T600	R601
L359	L360	T361	G362	L365	Q366	N367	S370	E371	L372	W373	S374	L375	C376	N377	F378	D501	L380	P381	D382	L383	F384	T385	S386	H387	D388	E389	F390	E391	S392	W393	F394	D395	PHE	SER	GLU	LYS	ASN	LYS	ASN	GLU	ALA	THR	LYS	E407	E408	E409	E410	K411	R412	R413	A414	Q415	V416	V417	S418	K419	L420	
L421	G422	I423	L424	R425	P426	F427	I428	L429	R430	R431	M432	K433	C434	D435	V436	E437	L438	S439	L440	P441	R442	K443	K444	E445	I446	I447	M448	Y449	A450	T451	M452	T453	D454	H455	Q456	K457	K458	F459	Q460	E461	H462	L463	V464	N465	H466	F467	L468	E469	H471	L472	G473	E474	M475	A476	ILE	ARG	GLY	GLN
GLY	TRP	LYS	GLY	K485	L486	N487	N488	L489	V490	I491	Q492	L493	R494	K495	N498	H499	P500	D501	L502	L503	Q504	Q506	I507	D508	G509	S510	Y511	L512	Y513	P514	P515	V516	E517	E518	I519	V520	Q521	Q522	C523	G524	K525	F526	R527	L528	L529	E530	R531	L532	L533	V534	R535	L536	F537	A538	N539	M540	H541	
K542	V543	L544	I545	F546	S547	Q548	T550	K551	L552	L553	D554	I555	M556	D557	Y558	Y559	F560	S561	E562	K563	G564	F565	E566	V567	C568	R569	I570	D571	G572	S573	V574	K575	L576	D577	E578	R579	R580	R581	Q582	I583	K584	D585	F586	S587	D588	E589	K590	S591	S592	C593	S594	I595	F596	L597	L598	S599	T600	R601
A602	G603	G604	L605	G606	I607	Q608	L609	T610	A611	A612	D613	T614	C615	C616	L617	V618	D619	S620	D621	W622	N623	P624	Q625	M626	D627	L628	Q629	A630	I631	D632	G633	C634	H635	R636	I637	G638	Q639	T640	K641	P642	V643	H644	V645	Y646	D647	L648	S649	T650	A651	Q652	S653	I654	E655	T656	R657	R661	A662	Y663
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
SER	ASP	LEU	THR	ILE	THR	ALA	PRO	GLY	THR	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																				
E184	T185	V186	I187	K188	L189	Q190	N191	E192	L193	C194	P195	L196	L197	T198	G199	Q200	Q201	L202	L203	S204	Q205	Q206	K208	G209	V210	K211	W212	L213	L214	S215	L216	W217	Q218	N219	G220	L221	W222	G223	L224	L225	A226	D227	Q228	W229	G230	L231	G232	K233	T234	L235	Q236	T237						
L238	G239	F240	L241	S242	H243	L244	K245	V246	N247	G248	L249	D250	E251	P252	Y253	L254	V255	L256	A257	P258	L259	S260	L261	L262	S263	F266	H267	E268	L269	A270	R271	T272	T273	F274	S275	I276	N277	A278	L279	I280	Y281	H282	G283	D284	K285	N286	Q287	R288	D289	E290	L291	R292	R293	K294	H295	L296	P297	K298
T299	V300	G301	P302	K303	F304	P305	L306	V307	I308	T309	Y311	E312	V313	P314	M315	N316	D317	A318	K319	R320	L321	S322	R323	H324	Y325	P326	W327	K328	Y329	V330	V331	L332	D333	E334	S335	H336	R337	L338	K339	N340	H341	K342	C343	K344	L345	L346	R347	E348	L349	K350	H351	L352	K353	H354	D355	N356	K357	L358
L359	L360	T361	G362	L365	Q366	N367	S370	E371	L372	W373	S374	L375	C376	N377	F378	D501	L380	P381	D382	L383	F384	T385	S386	H387	D388	E389	F390	E391	S392	W393	F394	D395	PHE	SER	GLU	LYS	ASN	LYS	ASN	GLU	ALA	THR	LYS	E407	E408	E409	E410	K411	R412	R413	A414	Q415	V416	V417	S418	K419	L420	
H421	G422	I423	L424	R425	P426	F427	I428	L429	R430	R431	M432	K433	C434	D435	V436	E437	L438	S439	L440	P441	R442	K443	K444	E445	I446	I447	M448	Y449	A450	T451	M452	T453	D454	H455	Q456	K457	K458	F459	Q460	E461	H462	L463	V464	N465	H466	F467	L468	E469	H471	L472	G473	E474	M475	A476	ILE	ARG	GLY	GLN
GLY	TRP	LYS	GLY	K485	L486	N487	N488	L489	V490	I491	Q492	L493	R494	K495	N498	H499	P500	D501	L502	L503	Q504	Q506	I507	D508	G509	S510	Y511	L512	Y513	P514	P515	V516	E517	E518	I519	V520	Q521	Q522	C523	G524	K525	F526	R527	L528	L529	E530	R531	L532	L533	V534	R535	L536	F537	A538	N539	M540	H541	
K542	V543	L544	I545	F546	S547	Q548	T550	K551	L552	L553	D554	I555	M556	D557	Y558	Y559	F560	S561	E562	K563	G564	F565	E566	V567	C568	R569	I570	D571	G572	S573	V574	K575	L576	D577	E578	R579	R580	R581	Q582	I583	K584	D585	F586	S587	D588	E589	K590	S591	S592	C593	S594	I595	F596	L597	L598	S599	T600	R601
A602	G603	G604	L605	G606	I607	Q608	L609	T610	A611	A612	D613	T614	C615	C616	L617	V618	D619	S620	D621	W622	N623	P624	Q625	M626	D627	L628	Q629	A630	I631	D632	G633	C634	H635	R636	I637	G638	Q639	T640	K641	P642	V643	H644	V645	Y646	D647	L648	S649	T650	A651	Q652	S653	I654	E655	T656	R657	R661	A662	Y663
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					
L666	K667	H670	V671	V672	I673	G674	Q675	GLY	GLN	ALA	ALA	GLU	PHE	ALA	PRO	V743	V744	G745	P746	G747	W748	W749	V750	V751	V752	P753	S754	S755	G756	G757	M758	LEU	SER	SER	LEU	ASN	SER																					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34559	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	10000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	211.99998, 211.99998, 211.99998	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.37	0/605	0.60	1/812 (0.1%)
1	E	0.20	0/628	0.49	0/842
2	B	0.36	0/643	0.59	3/861 (0.3%)
2	F	0.20	0/683	0.54	0/912
3	C	0.16	0/685	0.36	0/918
3	G	0.19	0/644	0.49	0/866
4	D	0.20	0/714	0.51	0/959
4	H	0.16	0/714	0.51	2/959 (0.2%)
5	I	0.23	0/2531	0.42	0/3900
6	J	0.21	0/2573	0.38	0/3973
7	K	0.28	0/4162	0.64	9/5611 (0.2%)
All	All	0.24	0/14582	0.51	15/20613 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	509	GLY	N-CA-C	-15.72	92.78	114.95
7	K	504	GLN	N-CA-C	-10.99	98.83	111.03
7	K	231	LEU	N-CA-C	-8.61	101.86	111.07
7	K	511	TYR	N-CA-C	-7.73	101.59	111.02
1	A	80	THR	N-CA-C	7.30	121.17	109.86

There are no chirality outliers.

There are no planarity outliers.

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	598	0	628	40	0
1	E	621	0	650	39	0
2	B	636	0	675	41	0
2	F	676	0	724	30	0
3	C	676	0	723	33	0
3	G	635	0	675	62	0
4	D	703	0	740	40	0
4	H	703	0	740	41	0
5	I	2260	0	1245	82	0
6	J	2291	0	1244	85	0
7	K	4082	0	4157	250	0
All	All	13881	0	12201	627	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 24.

The worst 5 of 627 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:G:47:ARG:NH2	3:G:51:ARG:HD2	1.32	1.43
3:G:47:ARG:HH22	3:G:51:ARG:CD	1.34	1.39
3:G:51:ARG:NH1	5:I:39:DA:H3'	1.41	1.35
7:K:505:GLY:HA2	7:K:508:ASP:OD2	1.22	1.31
7:K:505:GLY:CA	7:K:508:ASP:OD2	1.90	1.18

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	72/139 (52%)	70 (97%)	2 (3%)	0	100	100
1	E	75/139 (54%)	73 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	77/106 (73%)	74 (96%)	3 (4%)	0	100	100
2	F	82/106 (77%)	80 (98%)	2 (2%)	0	100	100
3	C	86/153 (56%)	85 (99%)	1 (1%)	0	100	100
3	G	80/153 (52%)	78 (98%)	2 (2%)	0	100	100
4	D	88/153 (58%)	87 (99%)	1 (1%)	0	100	100
4	H	88/153 (58%)	87 (99%)	1 (1%)	0	100	100
7	K	494/767 (64%)	459 (93%)	35 (7%)	0	100	100
All	All	1142/1869 (61%)	1093 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/111 (56%)	62 (100%)	0	100	100
1	E	64/111 (58%)	64 (100%)	0	100	100
2	B	65/81 (80%)	65 (100%)	0	100	100
2	F	69/81 (85%)	69 (100%)	0	100	100
3	C	67/119 (56%)	67 (100%)	0	100	100
3	G	63/119 (53%)	63 (100%)	0	100	100
4	D	79/126 (63%)	79 (100%)	0	100	100
4	H	79/126 (63%)	79 (100%)	0	100	100
7	K	454/679 (67%)	451 (99%)	3 (1%)	76	79
All	All	1002/1553 (64%)	999 (100%)	3 (0%)	84	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	K	231	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	K	436	VAL
7	K	504	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
7	K	456	GLN
7	K	582	GLN
7	K	675	GLN
7	K	488	ASN
7	K	228	GLN

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](#)

There are no chain breaks in this entry.

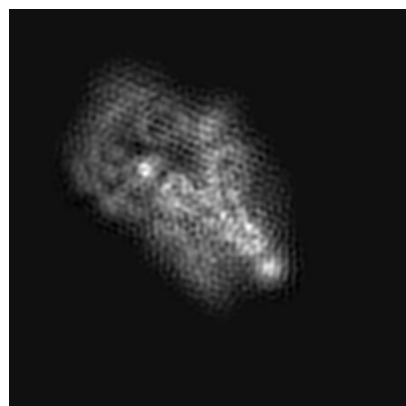
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36083. These allow visual inspection of the internal detail of the map and identification of artifacts.

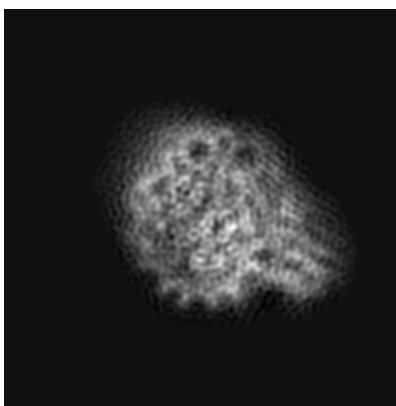
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

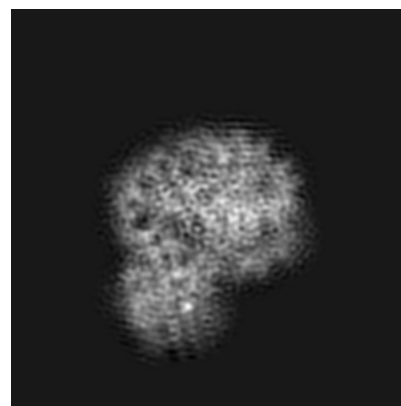
6.1.1 Primary map



X

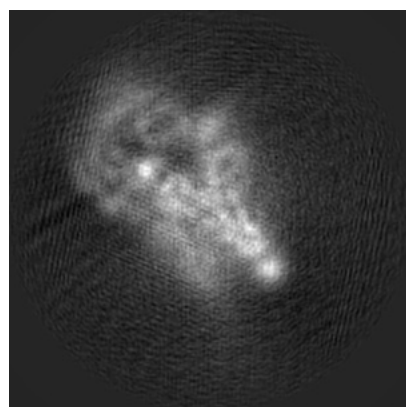


Y

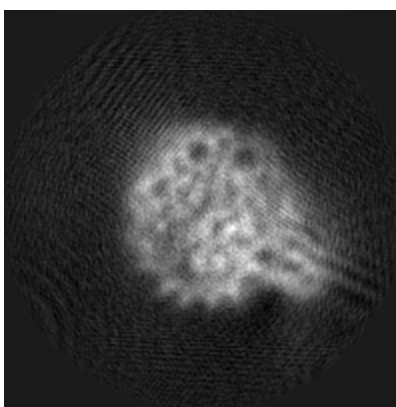


Z

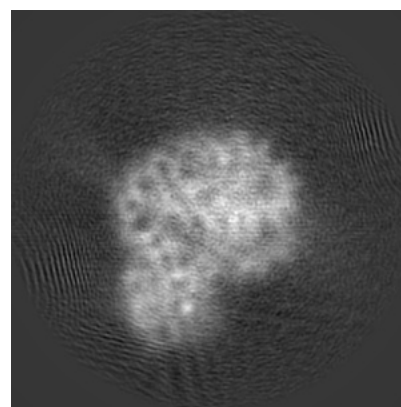
6.1.2 Raw map



X



Y

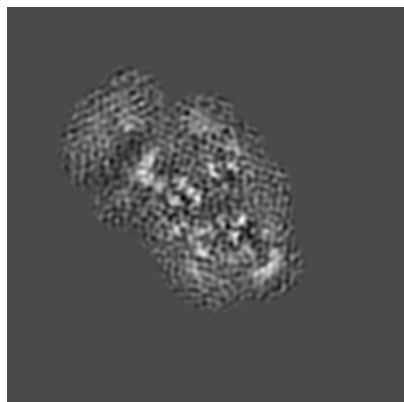


Z

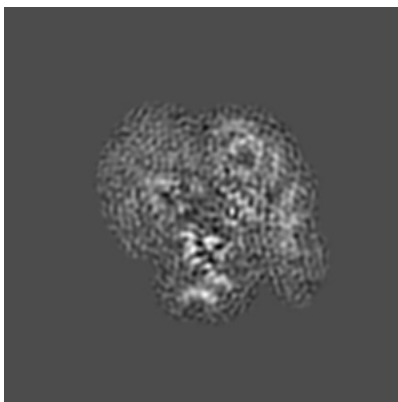
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

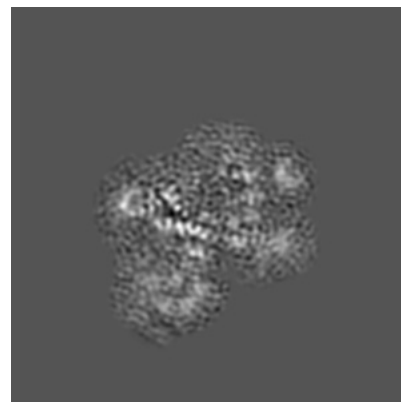
6.2.1 Primary map



X Index: 100

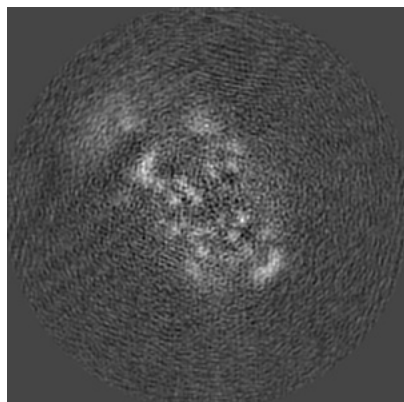


Y Index: 100

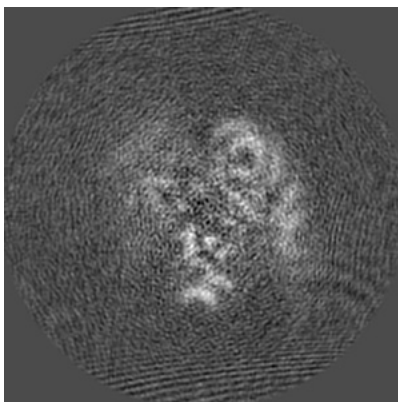


Z Index: 100

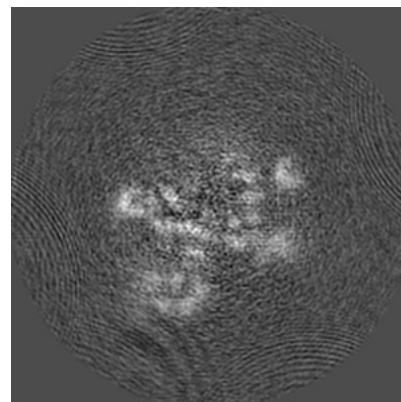
6.2.2 Raw map



X Index: 100



Y Index: 100

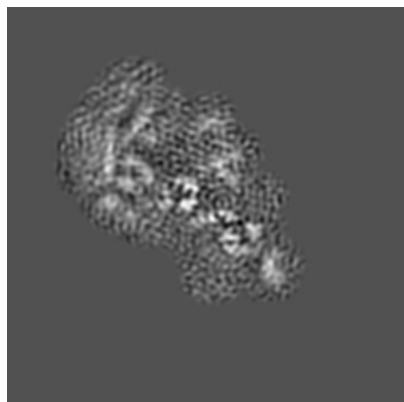


Z Index: 100

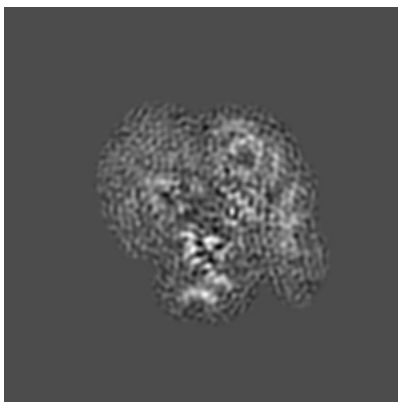
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

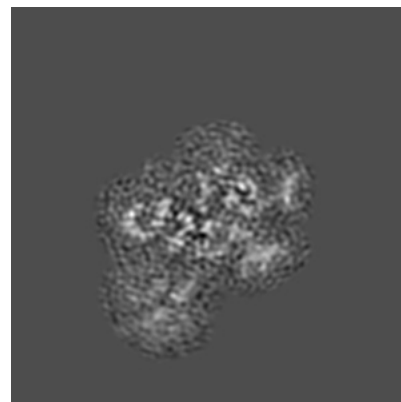
6.3.1 Primary map



X Index: 89

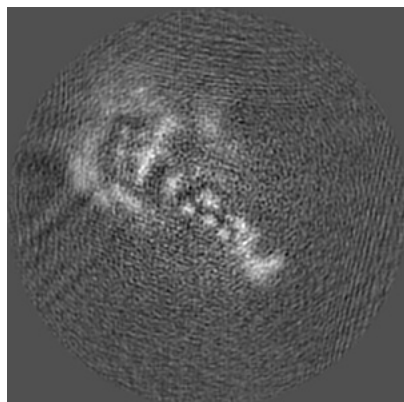


Y Index: 100

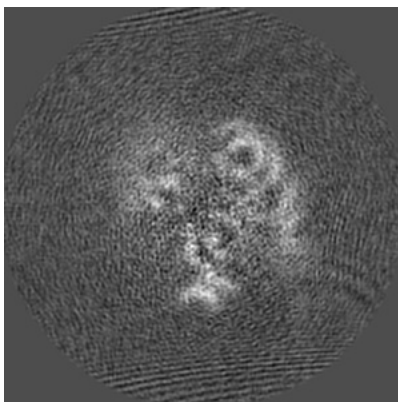


Z Index: 109

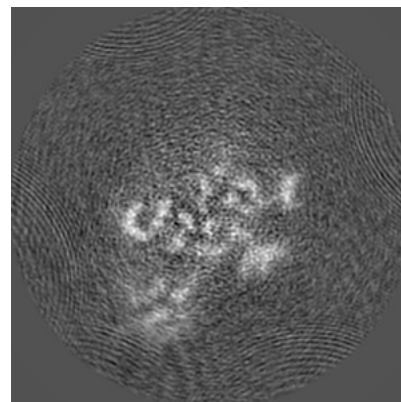
6.3.2 Raw map



X Index: 82



Y Index: 99

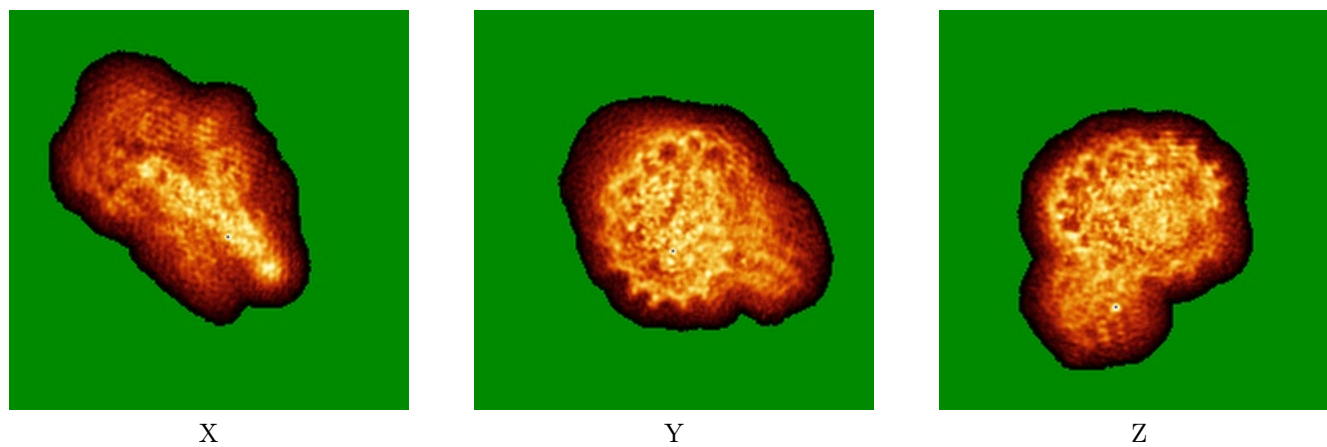


Z Index: 109

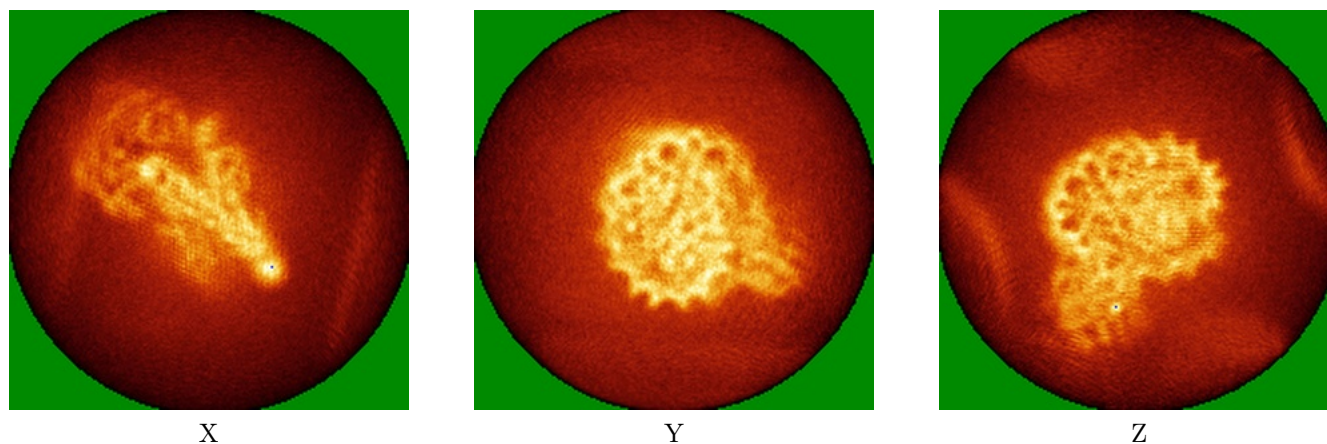
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

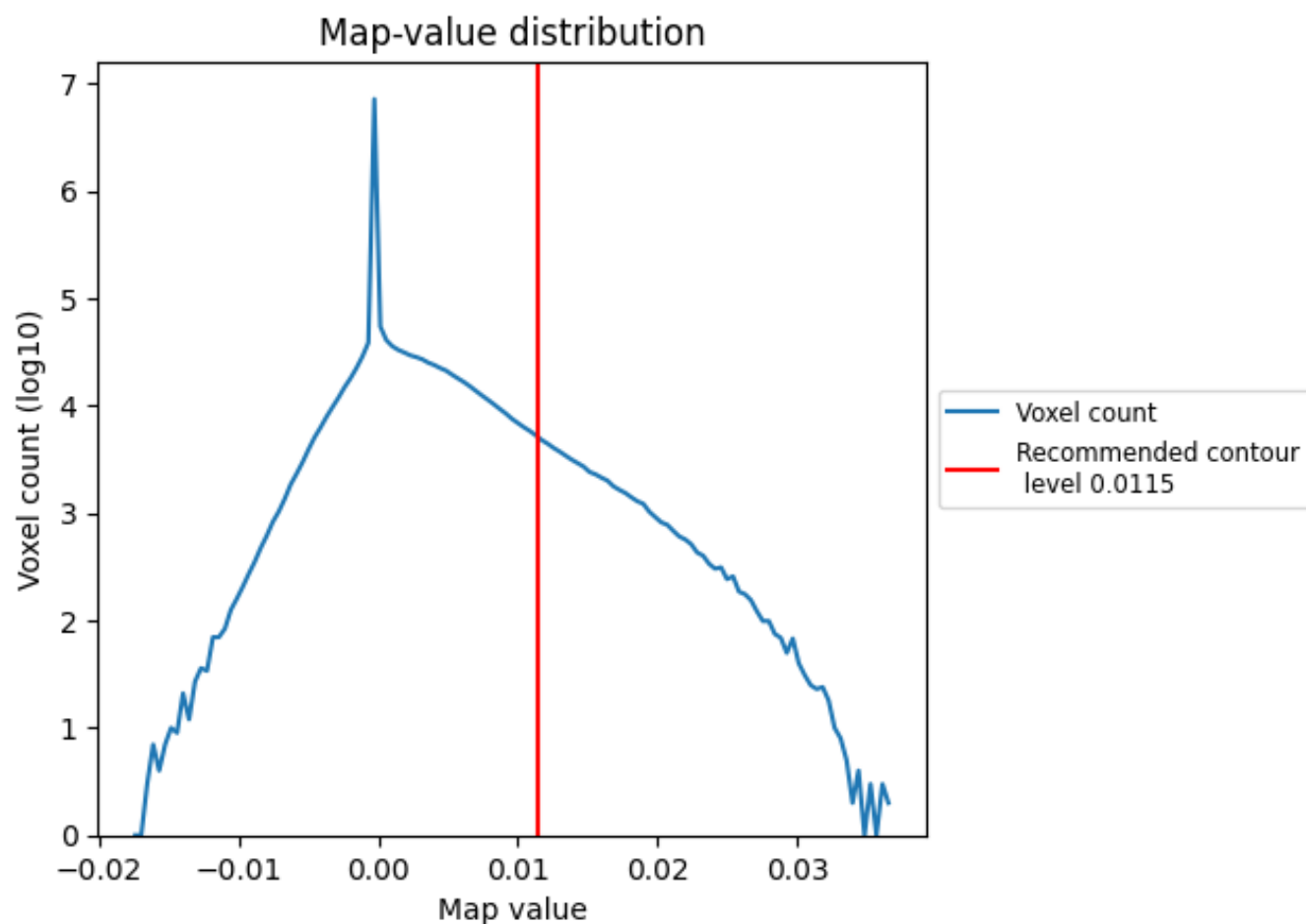
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

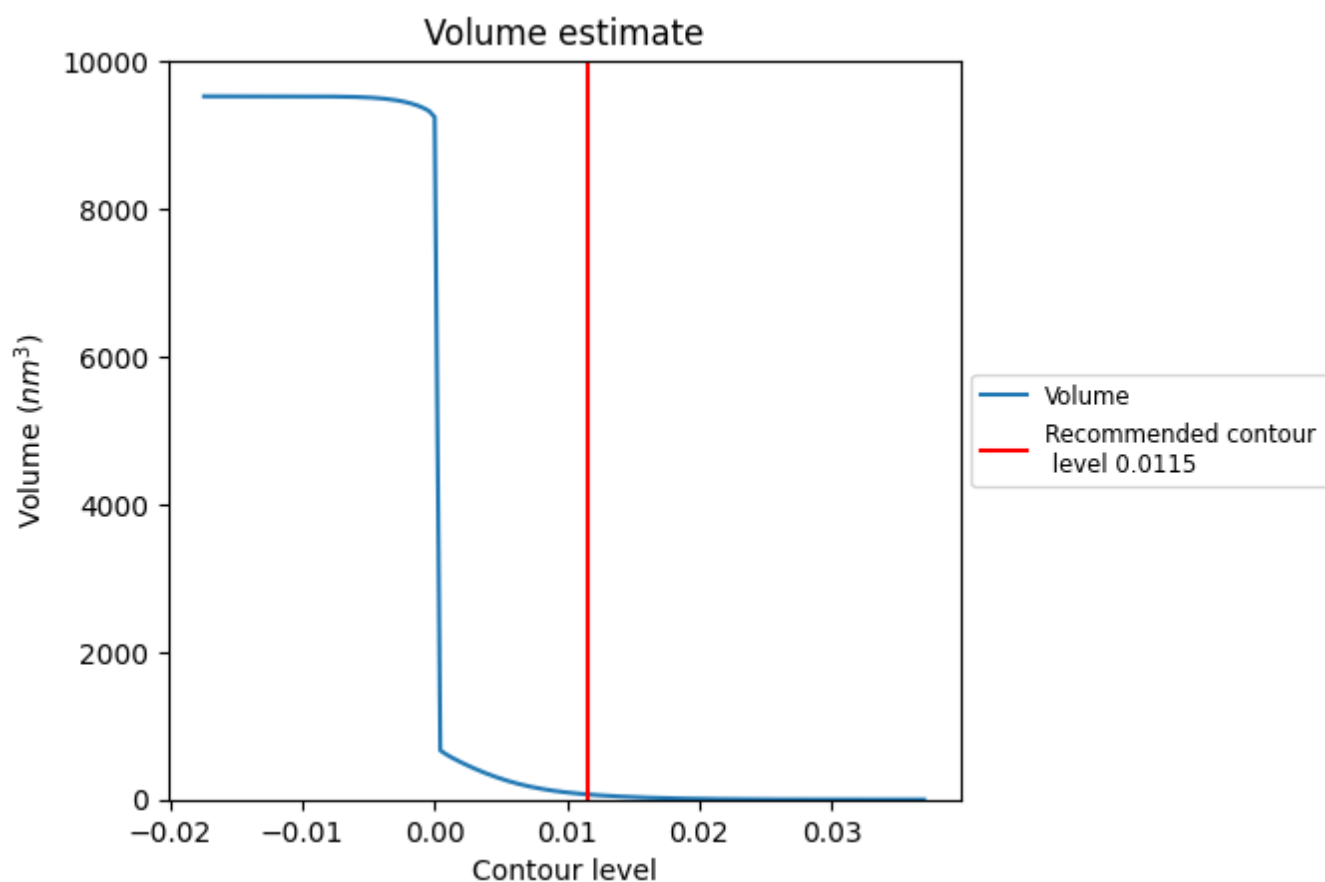
This section contains the results of statistical analysis of the map.

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.

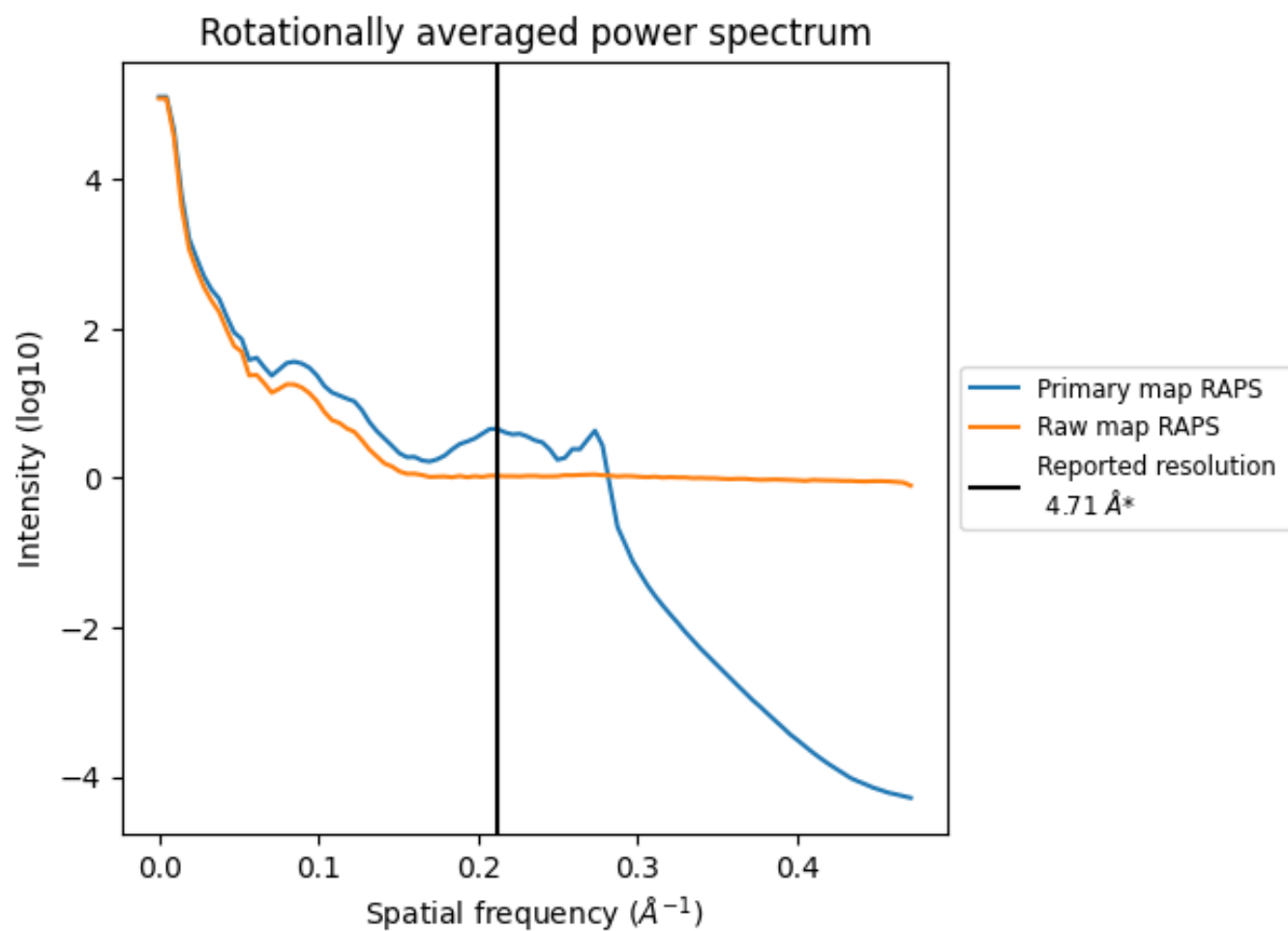
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm³; this corresponds to an approximate mass of 64 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 ⓘ

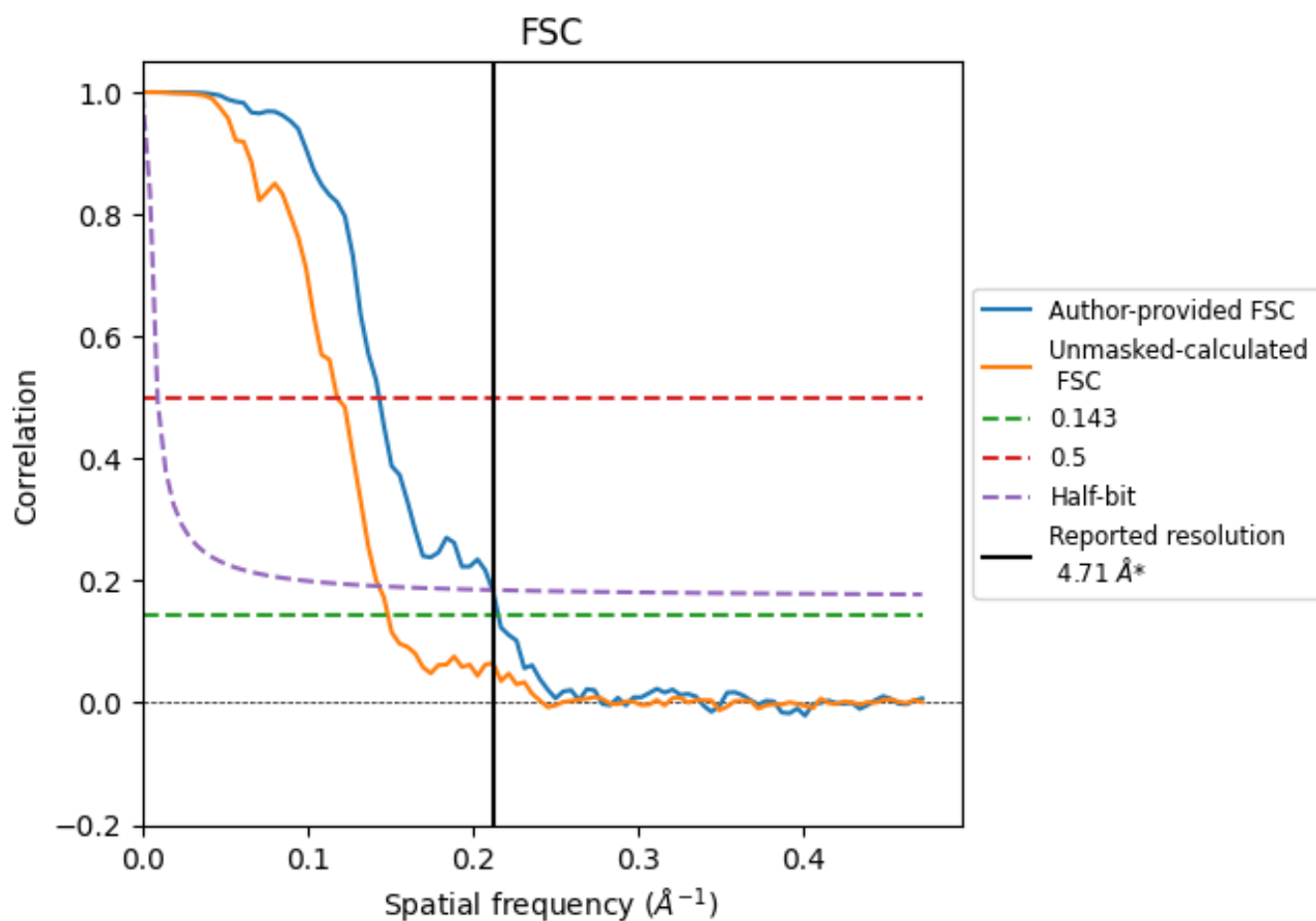


*Reported resolution corresponds to spatial frequency of 0.212 Å⁻¹

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 $0.212 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

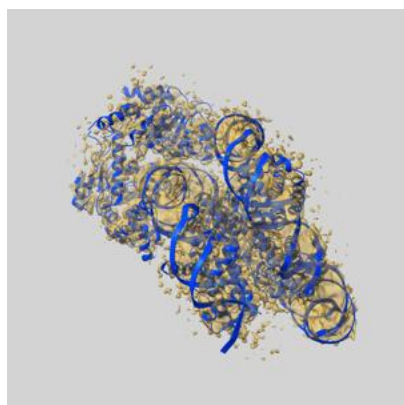
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.71	-	-
Author-provided FSC curve	4.64	6.98	4.72
Unmasked-calculated*	6.72	8.48	6.99

*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 6.72 differs from the reported value 4.71 by more than 10 %

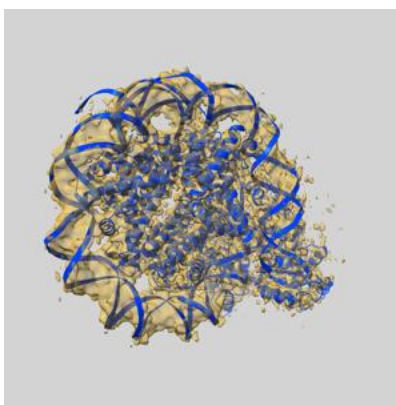
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36083 and PDB model 8J90. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

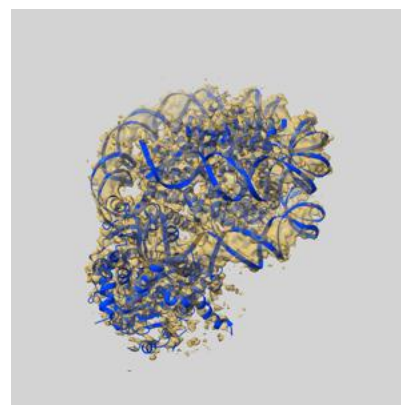
9.1 Map-model overlay [i](#)



X



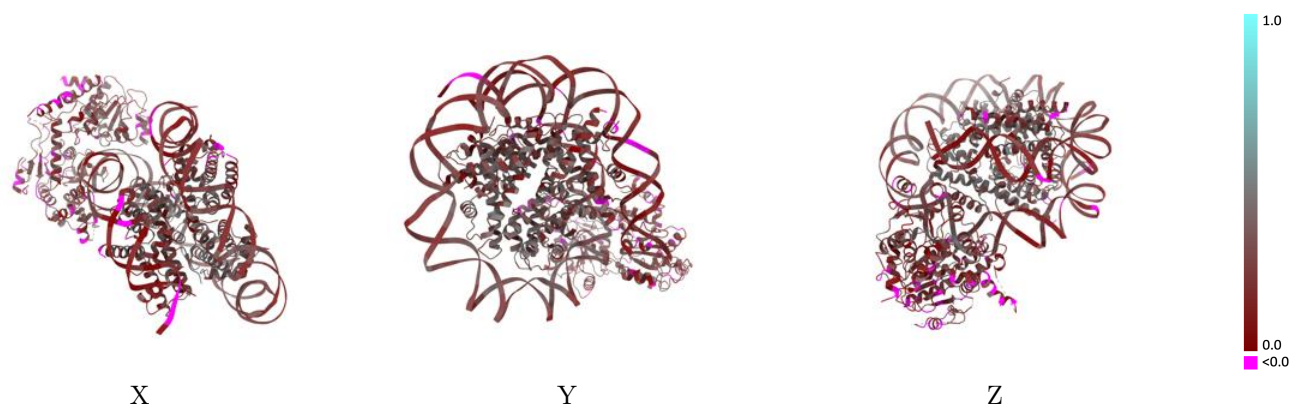
Y



Z

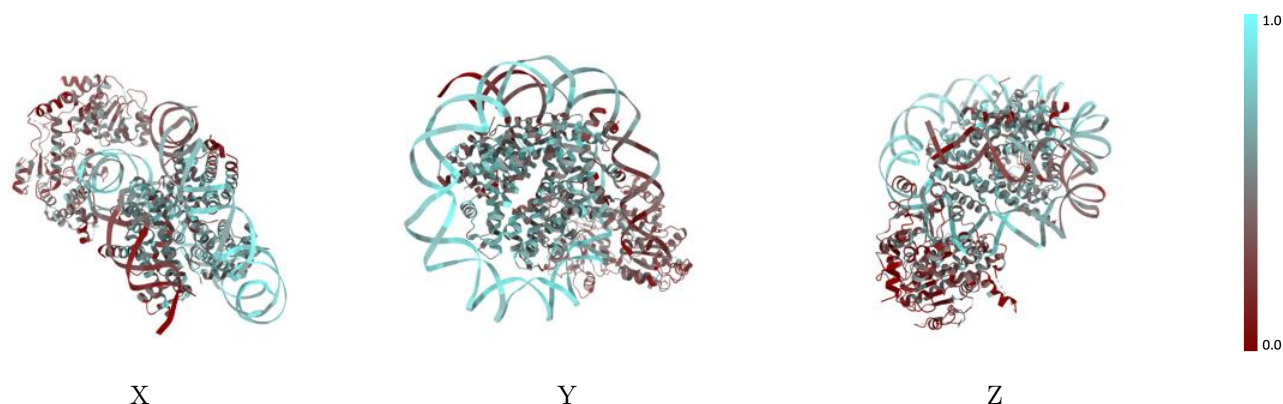
The images above show the 3D surface view of the map at the recommended contour level 0.0115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



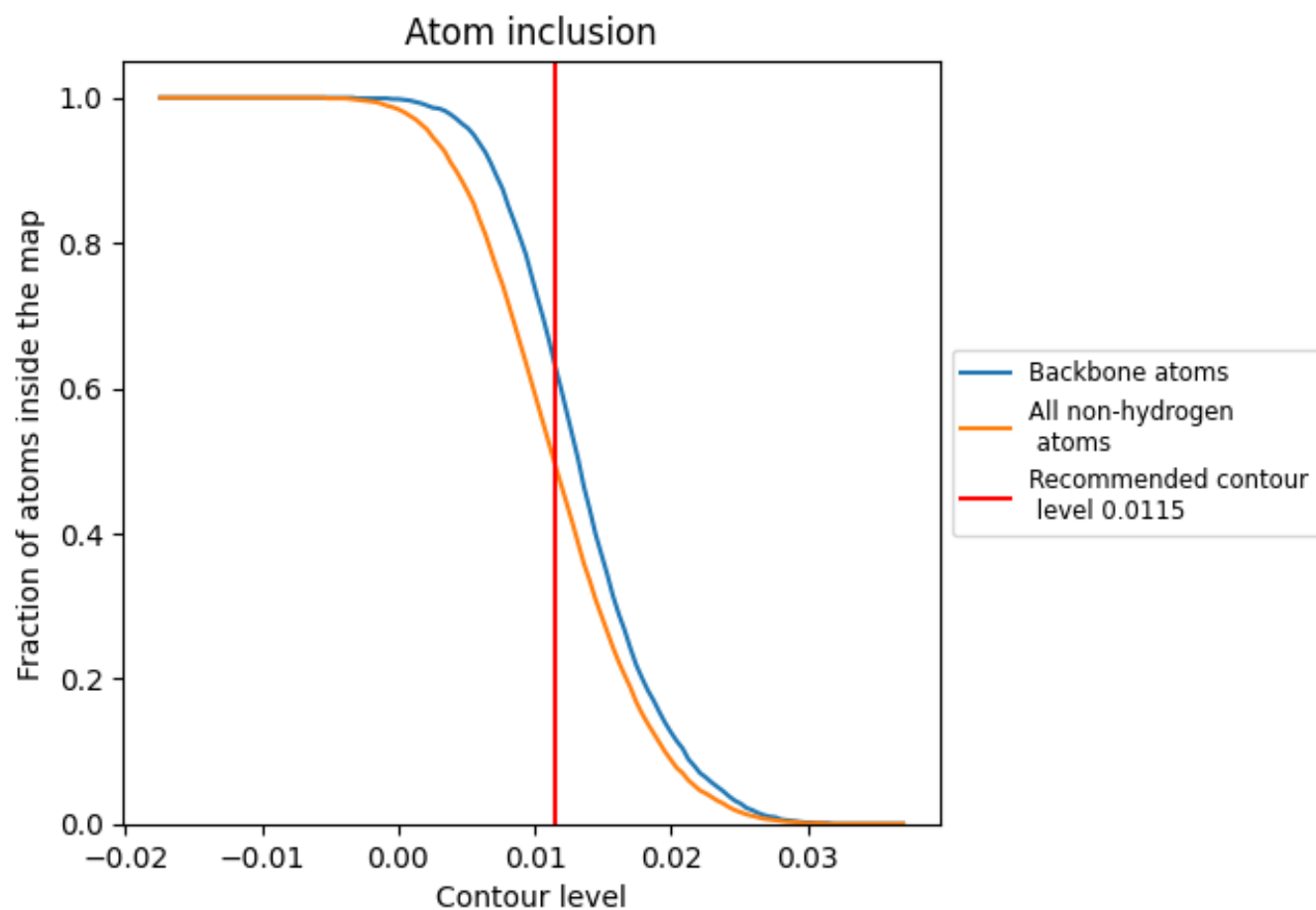
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0115).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 49% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4940	0.2430
A	0.6320	0.3540
B	0.6180	0.3480
C	0.4760	0.2630
D	0.4990	0.2700
E	0.5780	0.3240
F	0.5870	0.3220
G	0.4760	0.2500
H	0.5060	0.2590
I	0.6200	0.2310
J	0.6040	0.2260
K	0.2950	0.1890

1.0

0.0

<0.0