



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 09:31 AM UTC

PDB ID : 9Q9F / pdb_00009q9f
EMDB ID : EMD-52958
Title : DNA-PK bound to a 153 bp H2AX nucleosome model 1
Authors : Hall, C.; Chaplin, A.K.
Deposited on : 2025-02-26
Resolution : 4.54 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:

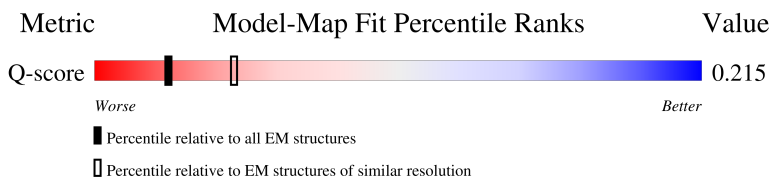
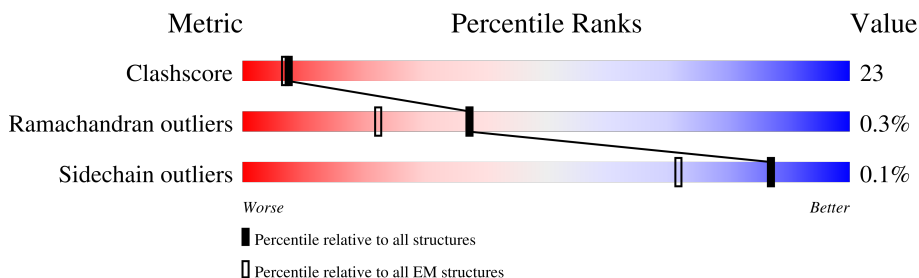
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.54 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	-
Q-score	-	25397	2475 (4.04 - 5.04)

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	K	609	
2	L	732	
3	I	153	
4	J	153	

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Mol	Chain	Length	Quality of chain
5	O	4128	
6	C	143	
6	G	143	
7	D	126	
7	H	126	
8	A	136	
8	E	136	
9	B	103	
9	F	103	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 46624 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	495	Total	C	N	O	S	0	0
			3926	2511	662	736	17		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	527	Total	C	N	O	S	0	0
			4165	2667	697	779	22		

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	129	Total	C	N	O	P	0	0
			2630	1247	481	773	129		

- Molecule 4 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	131	Total	C	N	O	P	0	0
			2697	1275	504	787	131		

- Molecule 5 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	3527	Total	C	N	O	S	0	0
			27830	17852	4683	5123	172		

- Molecule 6 is a protein called Histone H2AX.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	C	95	Total	C	N	O	0	0
			690	432	133	125		

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Mol	Chain	Residues	Atoms				AltConf	Trace
6	G	94	Total	C	N	O	0	0
			692	438	132	122		

- Molecule 7 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	93	Total	C	N	O	S	0	0
			719	450	130	137	2		
7	H	92	Total	C	N	O	S	0	0
			718	453	127	136	2		

- Molecule 8 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	88	Total	C	N	O	S	0	0
			697	442	128	123	4		
8	E	88	Total	C	N	O	S	0	0
			711	450	131	126	4		

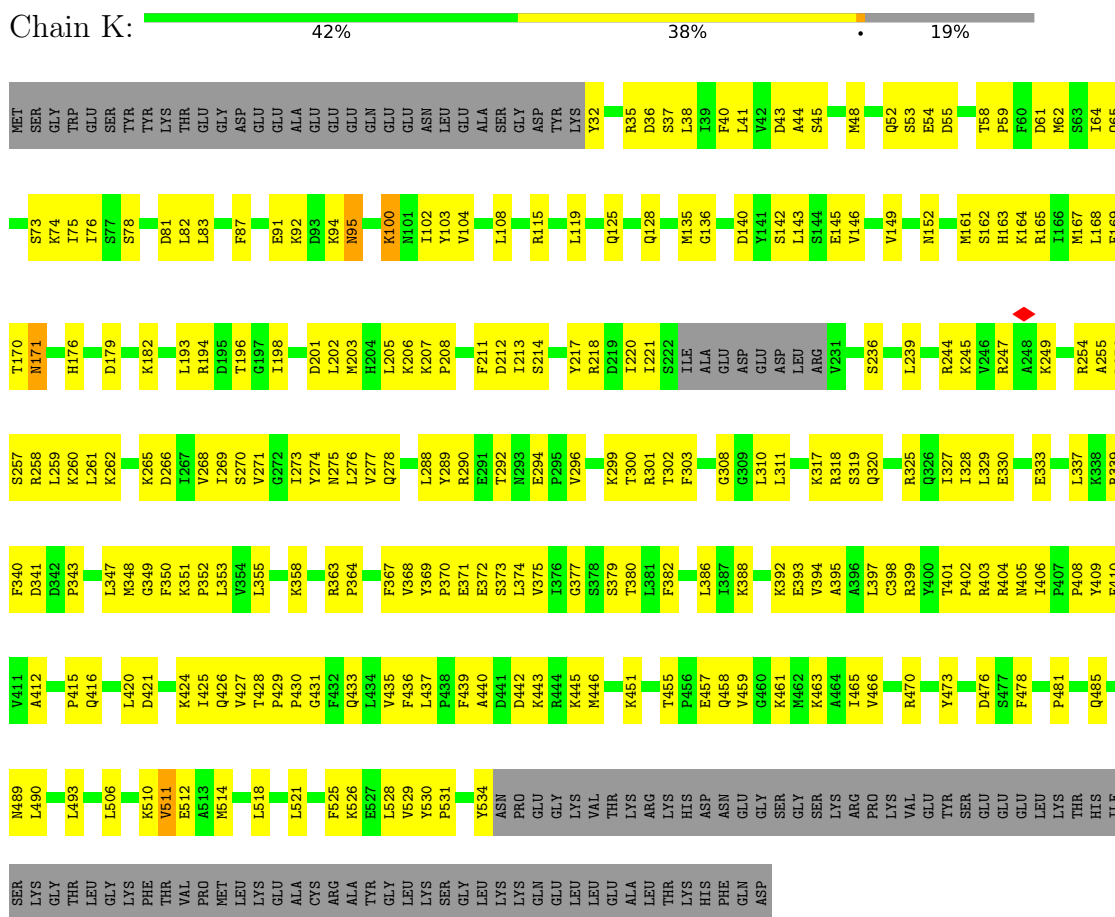
- Molecule 9 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	71	Total	C	N	O	S	0	0
			568	357	113	97	1		
9	F	72	Total	C	N	O	S	0	0
			581	370	112	98	1		

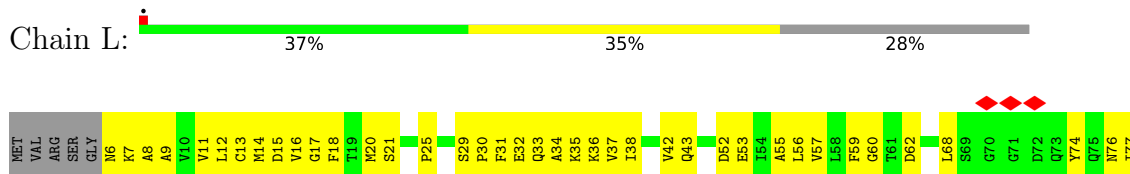
3 Residue-property plots

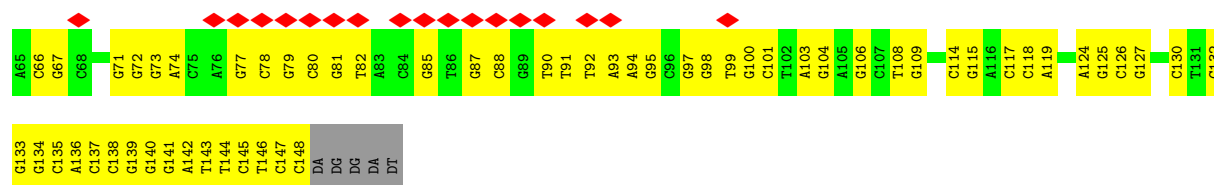
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: X-ray repair cross-complementing protein 6



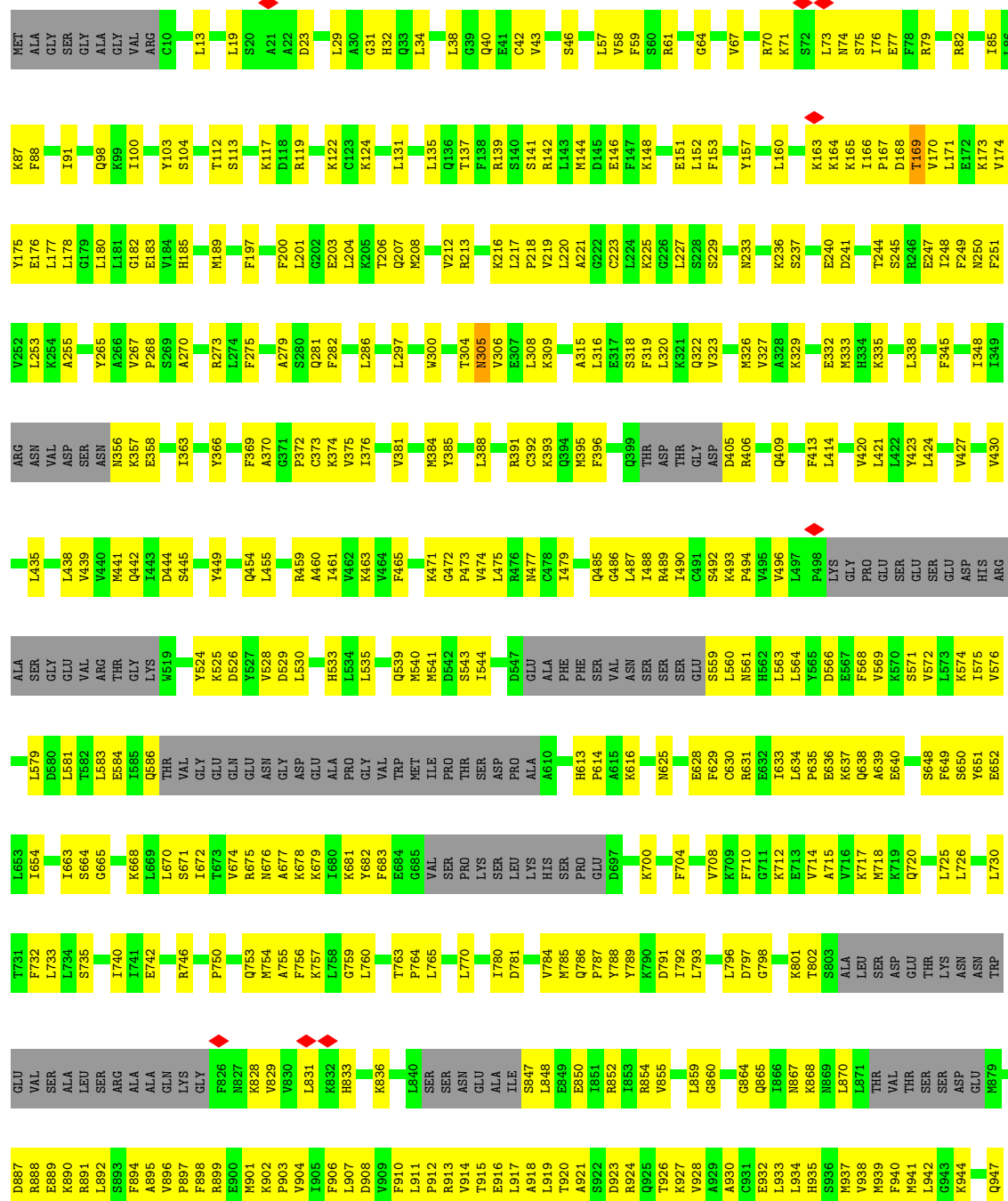
• Molecule 2: X-ray repair cross-complementing protein 5





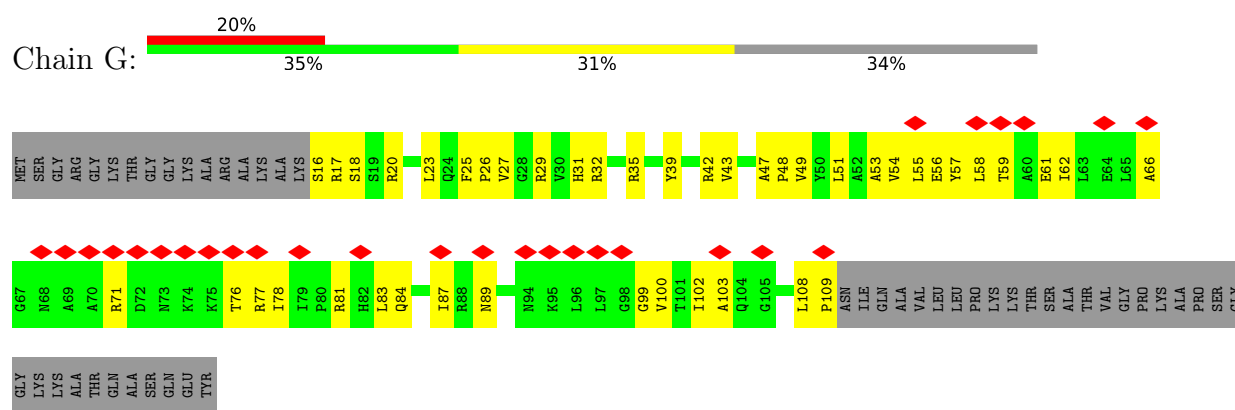
• Molecule 5: DNA-dependent protein kinase catalytic subunit

Chain O: 46% 39% 15%

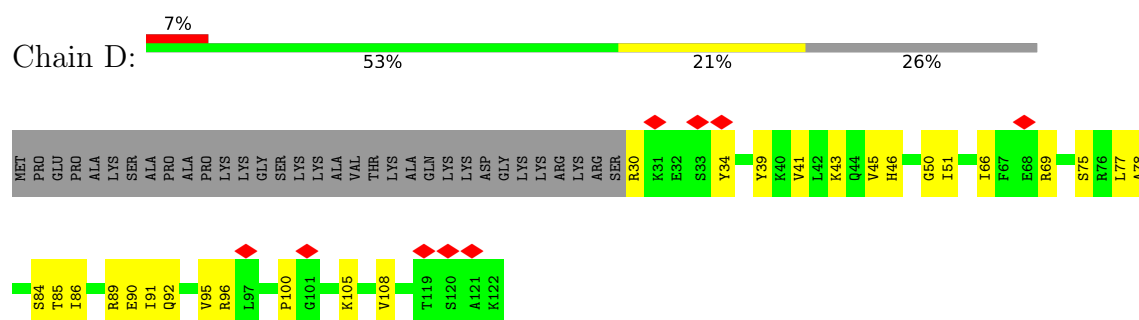




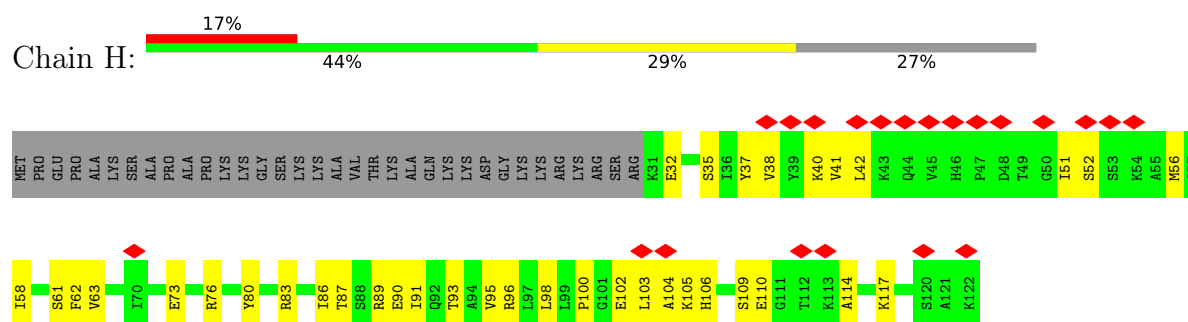
T3268	K3269	L3092	D3020	PRO	L2808	GLU	THR	T2535	C2435	N3665	P2284	D2208	P2136
R3270	D3271	A3099	S3021	P2918	G2815	LYS	LEU	L2536	I2438	K2366	L2285	L2211	I2137
W3272	D3273	K3100	ASN	D2919	E2819	SER	THR	R2537	P2139	V2367	C2292	R2214	V2138
L3273	Y3101	Y3102	PRO	W2923	Q2834	LEU	ARG	L2542	N2442	S3270	Q2295	L2215	L2140
L3274	L3103	I3103	ASP	E2925	K2835	THR	GLN	N2543	L2446	F3271	E2298	L2216	N2141
W3275	Q3104	Q3104	LEU	K2928	L2837	GLY	GLY	S2544	P2457	P2372	Y2299	F2218	L2142
Q3276	PRO	PRO	ASN	L2929	L2837	ARG	SER	L2545	F2373	L2374	Q2300	L2219	R2143
Q3277	GLU	I3107	I3030	K2936	Q2838	GLY	LEU	P2548	E2460	A2375	F2301	L2146	L2146
S3279	ASP	F3110	W3031	D2937	Q2839	VAL	SER	E2551	D2461	D2376	L2302	V2223	L2149
R3282	SER	Y3114	E3033	Y2936	F2840	ALA	ALA	E2552	V2462	R2377	L2303	P2224	P2250
L3283	MET	D3118	P3034	V2938	N2841	GLU	ARG	H2553	S2463	R2377	L2304	H2225	L2151
S3284	ASN	D3119	F3035	L2939	R2842	GLN	THR	P2554	H2464	M2379	N2305	P2226	I2152
H3285	VAL	V3119	F3036	L2942	T2847	LYS	PRO	S2556	P2465	N2380	N2306	K2227	T2153
C3286	ASP	Q3037	Q3037	I2942	F2848	ARG	ALA	L2557	S2466	A2381	F2309	R2228	E2154
R3287	GLN	R3125	E3038	K2950	F2851	GLY	ALA	A2558	T2467	V2382	V2310	V2230	E2155
S3288	ASP	K3128	T3039	L2957	F2852	LYS	LEU	T2559	R2470	L2385	R2311	F2231	V2156
R3289	GLY	L3129	M3044	L2957	P2852	ILE	GLN	N2560	E2471	K2388	R2158	R2232	F2157
S3290	ASP	L3129	I3045	A2961	F2853	SER	VAL	E2564	Q2472	A2317	P2159	H2233	P2159
Q3291	PRO	Q3133	K3046	D2973	F2854	GLY	ALA	M2565	N2473	G2391	A2318	N2234	V2160
S3294	SER	L3135	S3047	D2973	V2855	LEU	ASP	T2566	I2476	V2392	A2319	E2235	A2161
E3295	ARG	T3136	K3048	K2978	I2858	LYS	PHE	S2567	L2477	L2393	L2323	I2237	H2163
Q3296	MET	E3137	L3049	Q2979	C2863	MET	GLN	D2571	I2480	K2394	G2324	I2238	W2164
V3297	GLU	I3138	K3050	D2980	Q2864	LYS	HIS	Y2572	P2485	T2397	R2328	K2239	L2165
L3298	VAL	Q3139	L3051	L2984	L2868	ASP	PHE	N2574	D2486	R2485	V2329	P2252	S2166
T3299	GLN	Q3140	L3052	E2985	L2869	THR	LEU	S2582	PRO	V2400	V2330	P2252	P2167
V3300	GLY	F3141	K3054	E2985	L2869	GLY	LEU	F2586	GLU	E2403	M2331	S2250	L2169
L3301	GLN	F3142	Q3059	P2986	P2873	LEU	THR	T2587	GLU	G2407	E2332	K2259	Q2170
K3302	GLU	S3143	S3060	T2987	F2873	PRO	GLN	E2588	GLU	E2410	E2338	P2260	L2182
V3303	GLU	F3144	L3061	E2988	L2877	GLY	THR	Y2589	K2500	L2411	S2340	S2261	H2183
S3305	I3227	K3147	L3062	E2989	R2891	ASP	ALA	E2589	V2505	L2415	C2342	S2261	H2183
L3306	L3230	V3155	T3063	K2991	E2894	VAL	GLY	Y2590	L2510	D2419	E2343	D2264	V2186
E3309	F3236	F3156	F3064	D2992	E2895	ASP	ARG	T2591	I2511	F2420	L2344	P2265	V2187
V3312	K3241	K3157	K3067	F2993	A2896	ASN	THR	D2592	E2512	P2420	V2345	N2266	E2188
L3321	M3242	R3158	E3072	W2994	L2897	LYS	SER	D2593	F2413	F2413	S2340	S2267	L2189
A3322	D3244	L3161	L3073	L2996	L2898	VAL	PHE	S2594	L2415	L2415	C2342	S2261	V2190
R3324	S3245	N3162	Q3074	L2999	L2899	LYS	ASP	D2595	L2510	D2428	E2343	D2264	V2196
A3246	A3246	K3162	A3075	D3000	L2901	ALA	LEU	R2596	I2511	F2420	L2344	P2265	V2196
R3247	K3247	W3164	A3076	C3001	ALA	ALA	THR	F2597	E2512	P2421	V2345	N2266	E2188
Q3247	K3247	T3165	L3077	Y3002	LEU	SER	GLY	R2598	E2513	V2421	A2346	S2267	L2189
K3248	K3248	W3165	L3078	N3003	GLY	THR	THR	T2603	N2514	Q2422	C2342	S2267	V2190
Q3249	Q3249	P3169	H3081	H3004	PRO	ALA	ASP	PRO	L2517	V2423	L2349	N2270	K2191
L3328	L3329	P3175	Y3082	W3008	ALA	LYS	ASP	MET	Q2518	R2424	K2350	I2274	L2192
L3330	L3330	P3176	S3083	L3011	ARG	LYS	THR	PHE	Q2518	R2425	Q2351	I2274	L2193
G3331	G3331	M3176	Q3084	L3011	VAL	VAL	VAL	VAL	E2528	H2426	H2352	Q2275	L2194
T3332	T3332	W3179	E3085	C3014	ARG	GLY	ASP	GLU	T2529	R2427	Q2353	L2276	S2195
R3335	R3335	K3179	L3088	S3014	GLY	THR	HIS	THR	R2530	D2429	D2358	I2279	V2196
H3348	H3348	T3183	L3089	S3015	LYS	LYS	THR	GLN	R2530	D2429	K2359	V2280	A2200
K3267	K3267	R3186	Y3090	S3018	ALA	ARG	SER	ALA	P2552	R2431	F2360	M2281	A2281
			L3091	L3019	LEU	ARG	PRO	GLN	S2533	Q2432	I2361	V2205	V2205
							SER	GLY	N2534		V2362	N2283	



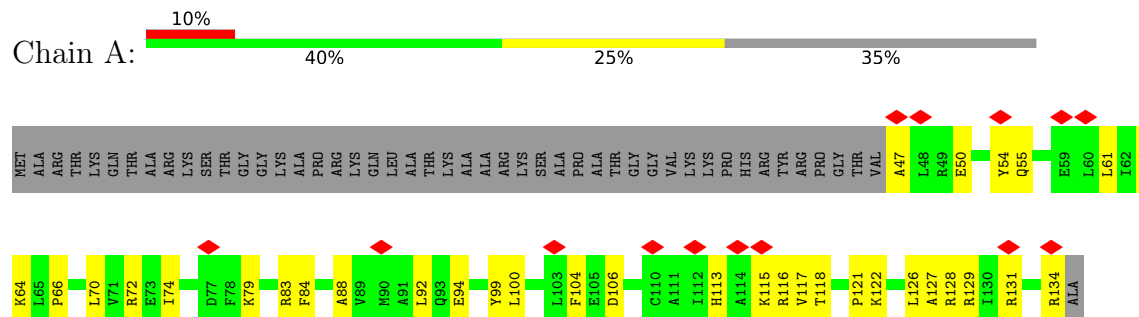
- Molecule 7: Histone H2B type 1-J



- Molecule 7: Histone H2B type 1-J

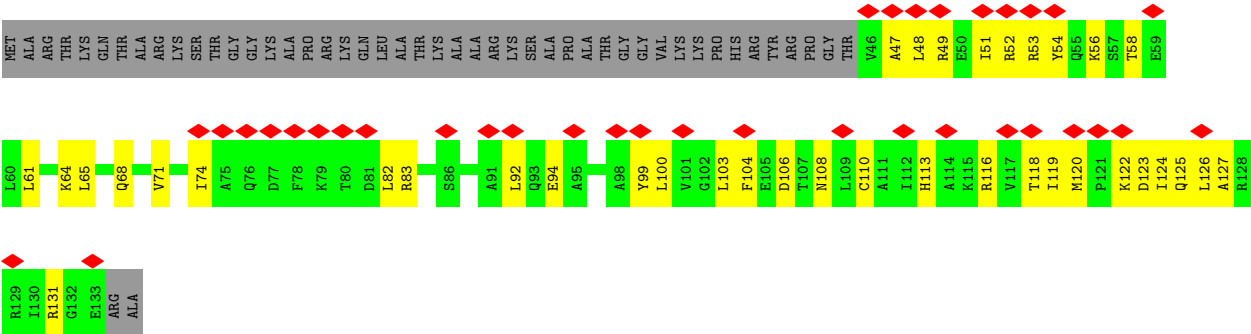


- Molecule 8: Histone H3.1

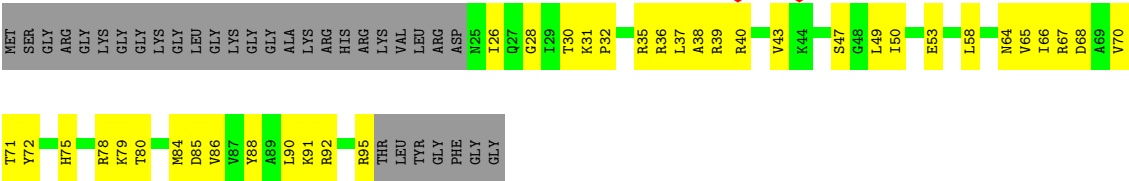


- Molecule 8: Histone H3.1

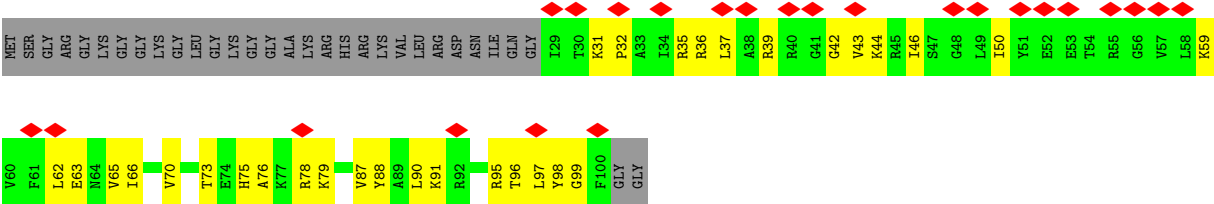




● Molecule 9: Histone H4



● Molecule 9: Histone H4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14174	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.59	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.839	Depositor
Minimum map value	-0.247	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	692.16, 692.16, 692.16	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6479999, 1.6479999, 1.6479999	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	K	0.10	0/4004	0.32	0/5409
2	L	0.12	0/4249	0.34	0/5742
3	I	0.18	0/2947	0.37	0/4542
4	J	0.17	0/3027	0.36	0/4673
5	O	0.14	0/28381	0.37	0/38396
6	C	0.12	0/700	0.33	0/951
6	G	0.14	0/702	0.42	0/951
7	D	0.11	0/729	0.31	0/980
7	H	0.13	0/729	0.38	0/979
8	A	0.10	0/705	0.31	0/948
8	E	0.18	0/719	0.41	0/966
9	B	0.11	0/573	0.28	0/767
9	F	0.14	0/588	0.38	0/788
All	All	0.14	0/48053	0.36	0/66092

There are no bond length outliers.

There are no bond angle outliers.

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	K	3926	0	3920	239	0
2	L	4165	0	4165	229	0
3	I	2630	0	1446	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	2697	0	1469	118	0
5	O	27830	0	27756	1243	0
6	C	690	0	676	42	0
6	G	692	0	704	57	0
7	D	719	0	735	23	0
7	H	718	0	740	42	0
8	A	697	0	710	46	0
8	E	711	0	737	44	0
9	B	568	0	614	39	0
9	F	581	0	625	40	0
All	All	46624	0	44297	2033	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 23.

The worst 5 of 2033 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)
5:O:965:THR:HG22	5:O:969:LEU:CD1	1.97	0.94
5:O:1633:TRP:HB2	5:O:1678:LEU:HD21	1.51	0.93
5:O:965:THR:HG22	5:O:969:LEU:HG	1.52	0.91
6:G:26:PRO:HB2	6:G:29:ARG:HB3	1.53	0.91
5:O:965:THR:HG22	5:O:969:LEU:CG	2.01	0.90

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	K	491/609 (81%)	438 (89%)	49 (10%)	4 (1%)	16	53
2	L	523/732 (71%)	471 (90%)	52 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	O	3455/4128 (84%)	3065 (89%)	379 (11%)	11 (0%)	36	71
6	C	93/143 (65%)	83 (89%)	9 (10%)	1 (1%)	11	45
6	G	92/143 (64%)	81 (88%)	11 (12%)	0	100	100
7	D	91/126 (72%)	88 (97%)	3 (3%)	0	100	100
7	H	90/126 (71%)	83 (92%)	7 (8%)	0	100	100
8	A	86/136 (63%)	82 (95%)	4 (5%)	0	100	100
8	E	86/136 (63%)	82 (95%)	4 (5%)	0	100	100
9	B	69/103 (67%)	68 (99%)	1 (1%)	0	100	100
9	F	70/103 (68%)	66 (94%)	4 (6%)	0	100	100
All	All	5146/6485 (79%)	4607 (90%)	523 (10%)	16 (0%)	37	71

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	O	2229	ALA
5	O	2535	THR
5	O	3295	GLU
5	O	3480	LEU
5	O	3855	TYR

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	K	432/548 (79%)	430 (100%)	2 (0%)	81	81
2	L	462/649 (71%)	462 (100%)	0	100	100
5	O	3042/3671 (83%)	3040 (100%)	2 (0%)	88	88
6	C	63/106 (59%)	63 (100%)	0	100	100
6	G	65/106 (61%)	65 (100%)	0	100	100
7	D	77/105 (73%)	77 (100%)	0	100	100
7	H	78/105 (74%)	78 (100%)	0	100	100

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Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	A	71/111 (64%)	71 (100%)	0	100	100
8	E	75/111 (68%)	75 (100%)	0	100	100
9	B	59/79 (75%)	59 (100%)	0	100	100
9	F	60/79 (76%)	60 (100%)	0	100	100
All	All	4484/5670 (79%)	4480 (100%)	4 (0%)	87	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	95	ASN
1	K	171	ASN
5	O	305	ASN
5	O	1961	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	458	GLN
5	O	1385	ASN
5	O	1926	ASN
5	O	2217	ASN
5	O	3470	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.

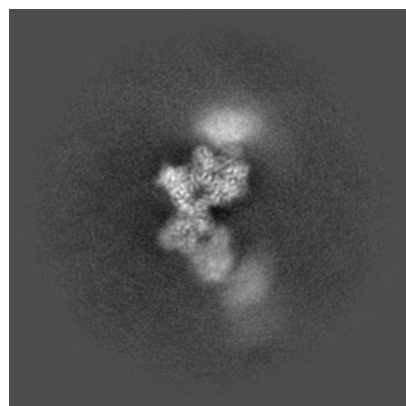
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52958. These allow visual inspection of the internal detail of the map and identification of artifacts.

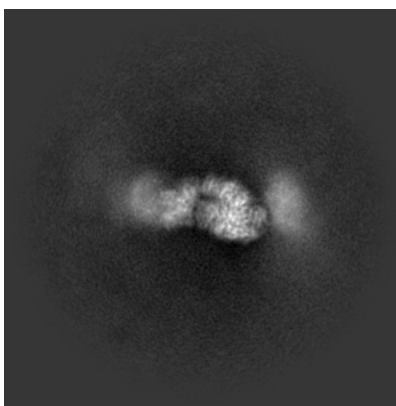
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

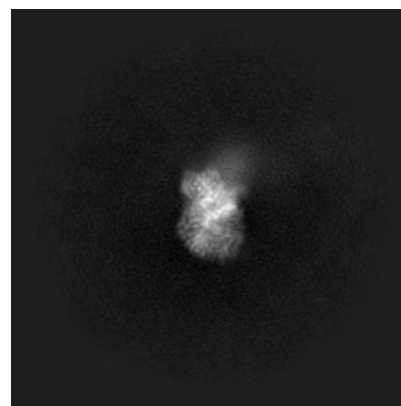
6.1.1 Primary map



X

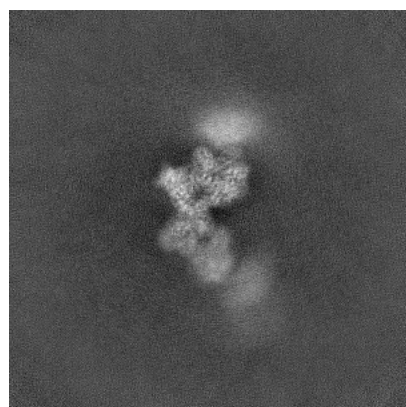


Y

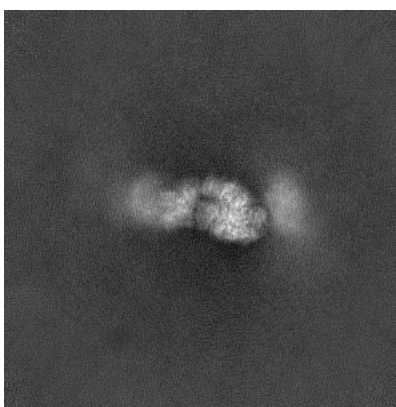


Z

6.1.2 Raw map



X



Y

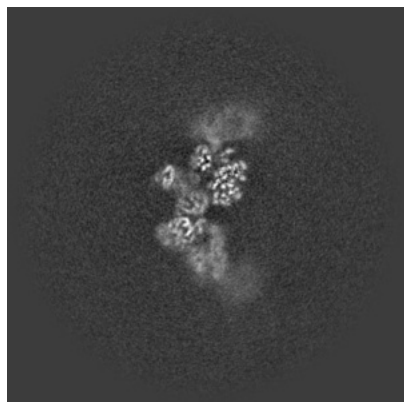


Z

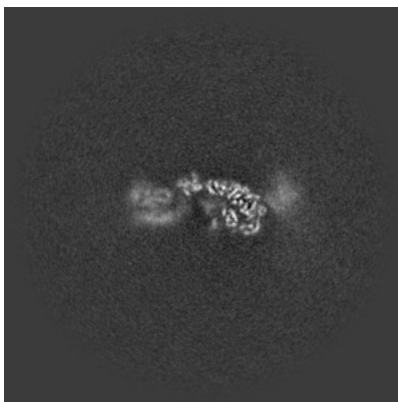
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

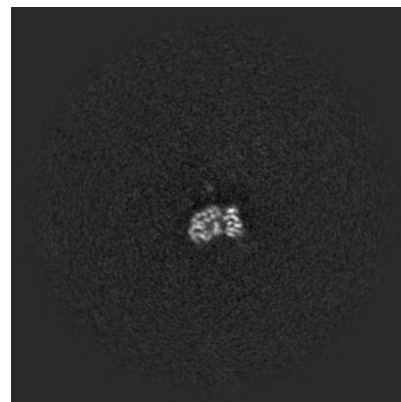
6.2.1 Primary map



X Index: 210

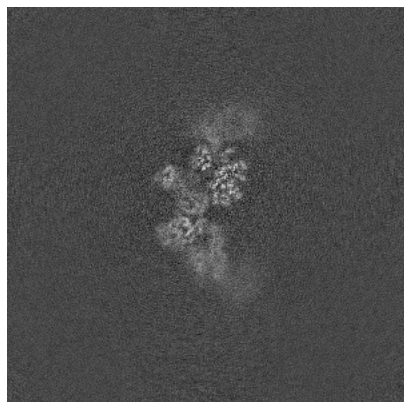


Y Index: 210



Z Index: 210

6.2.2 Raw map



X Index: 210



Y Index: 210

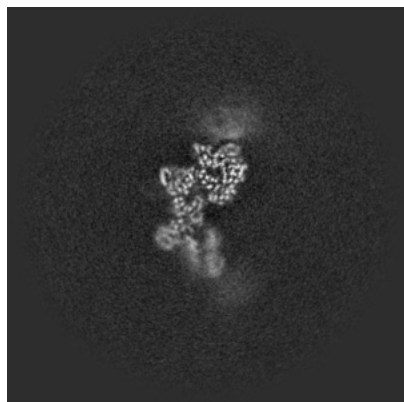


Z Index: 210

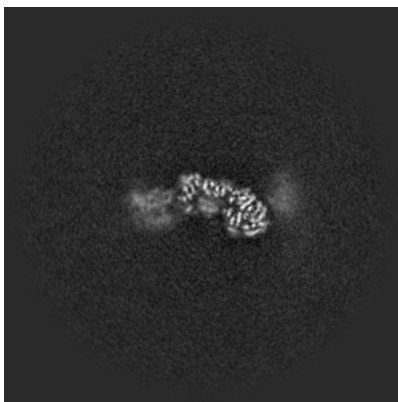
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

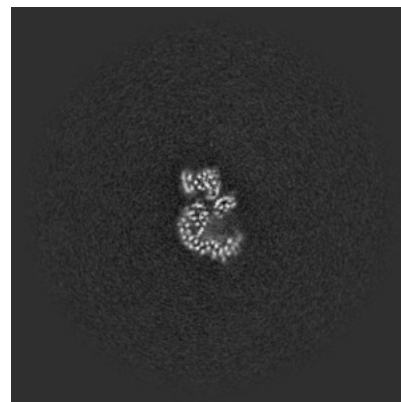
6.3.1 Primary map



X Index: 202



Y Index: 206



Z Index: 243

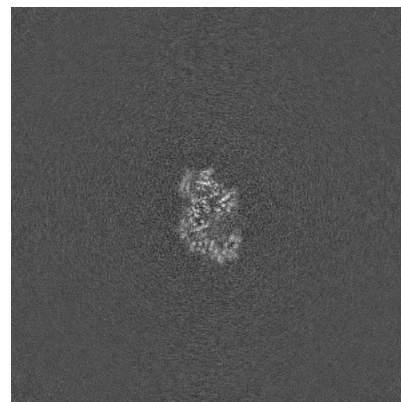
6.3.2 Raw map



X Index: 202



Y Index: 212

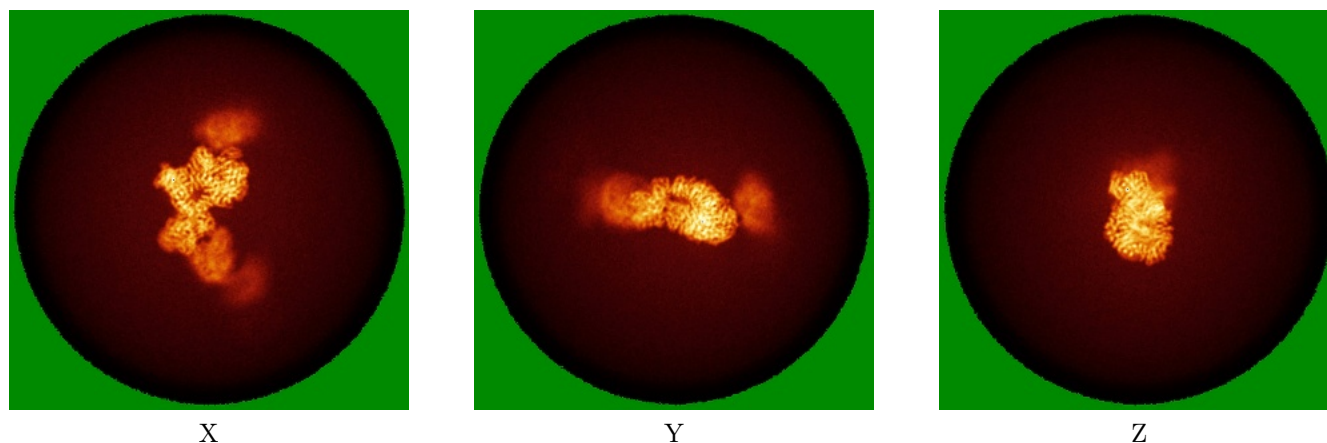


Z Index: 238

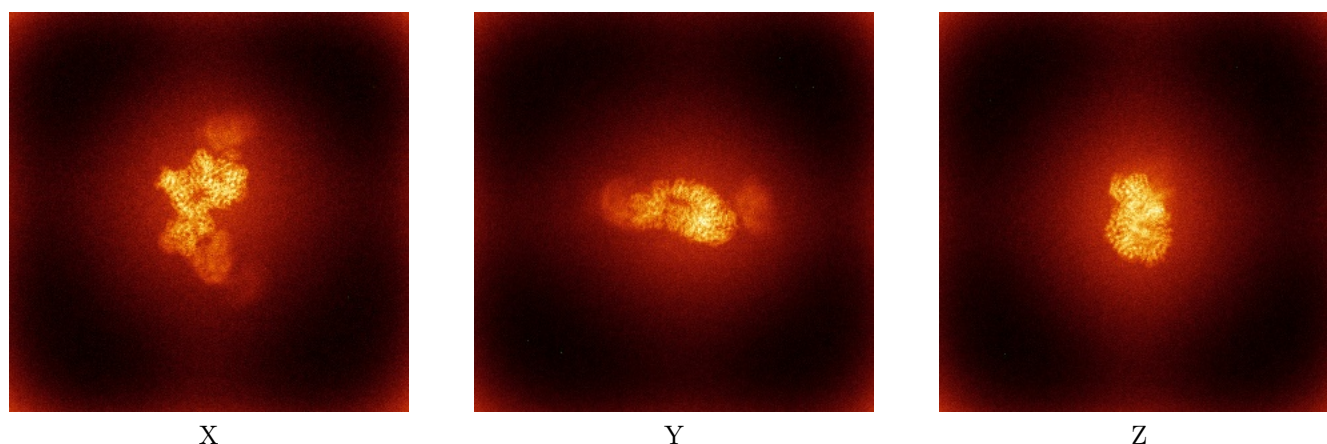
The images above show the largest variance slices of the map in three orthogonal directions.

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.

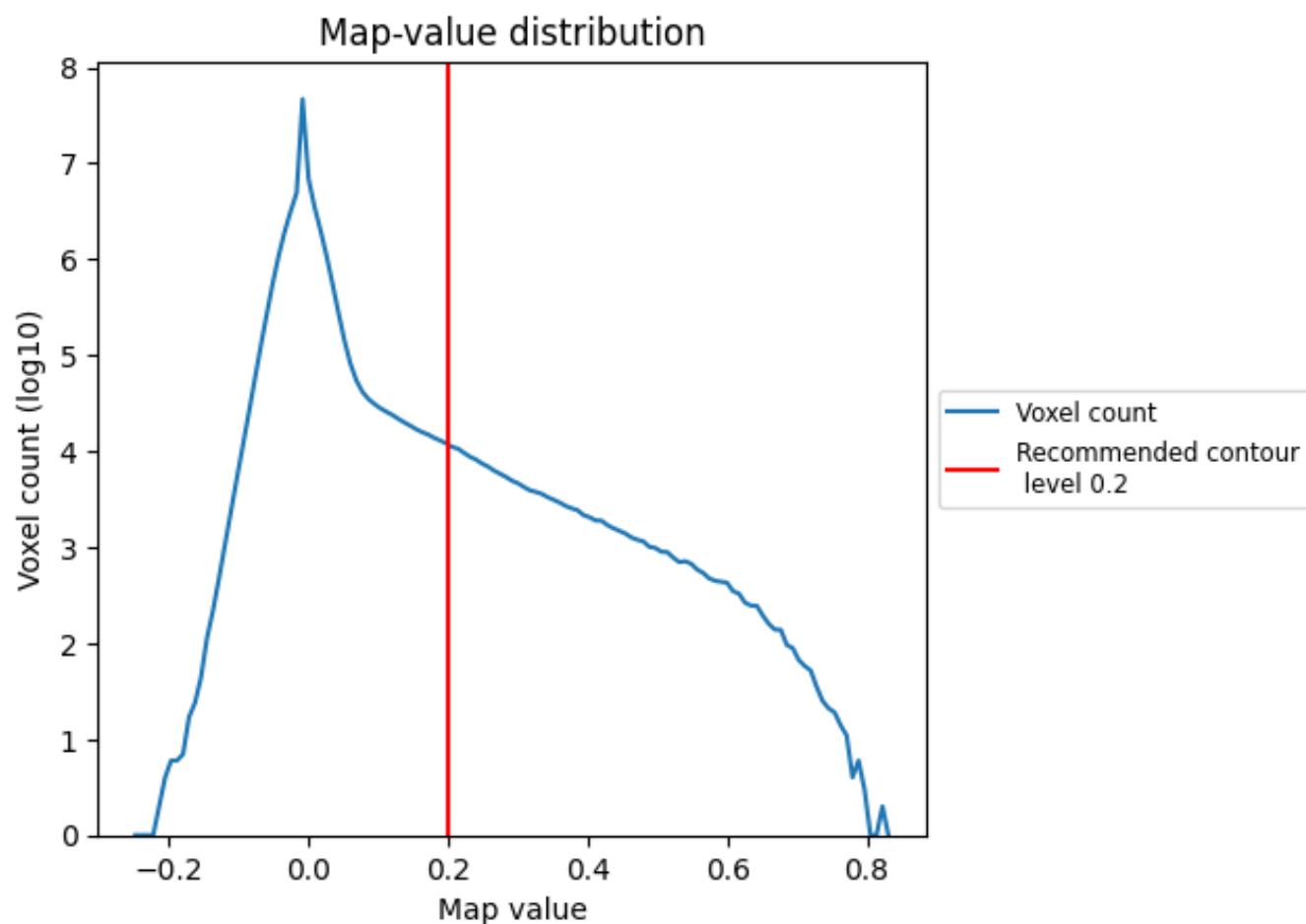
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

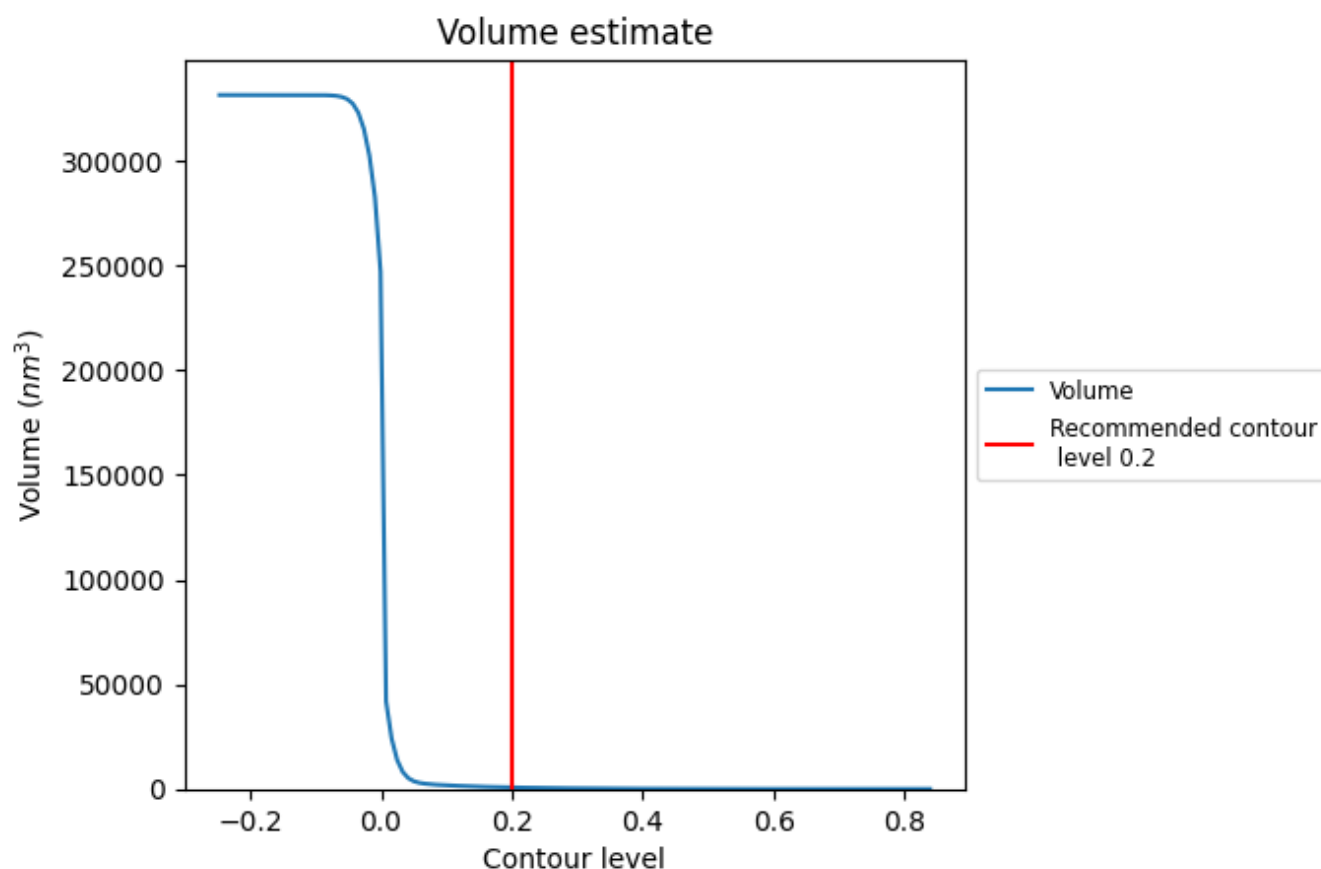
This section contains the results of statistical analysis of the map.

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.

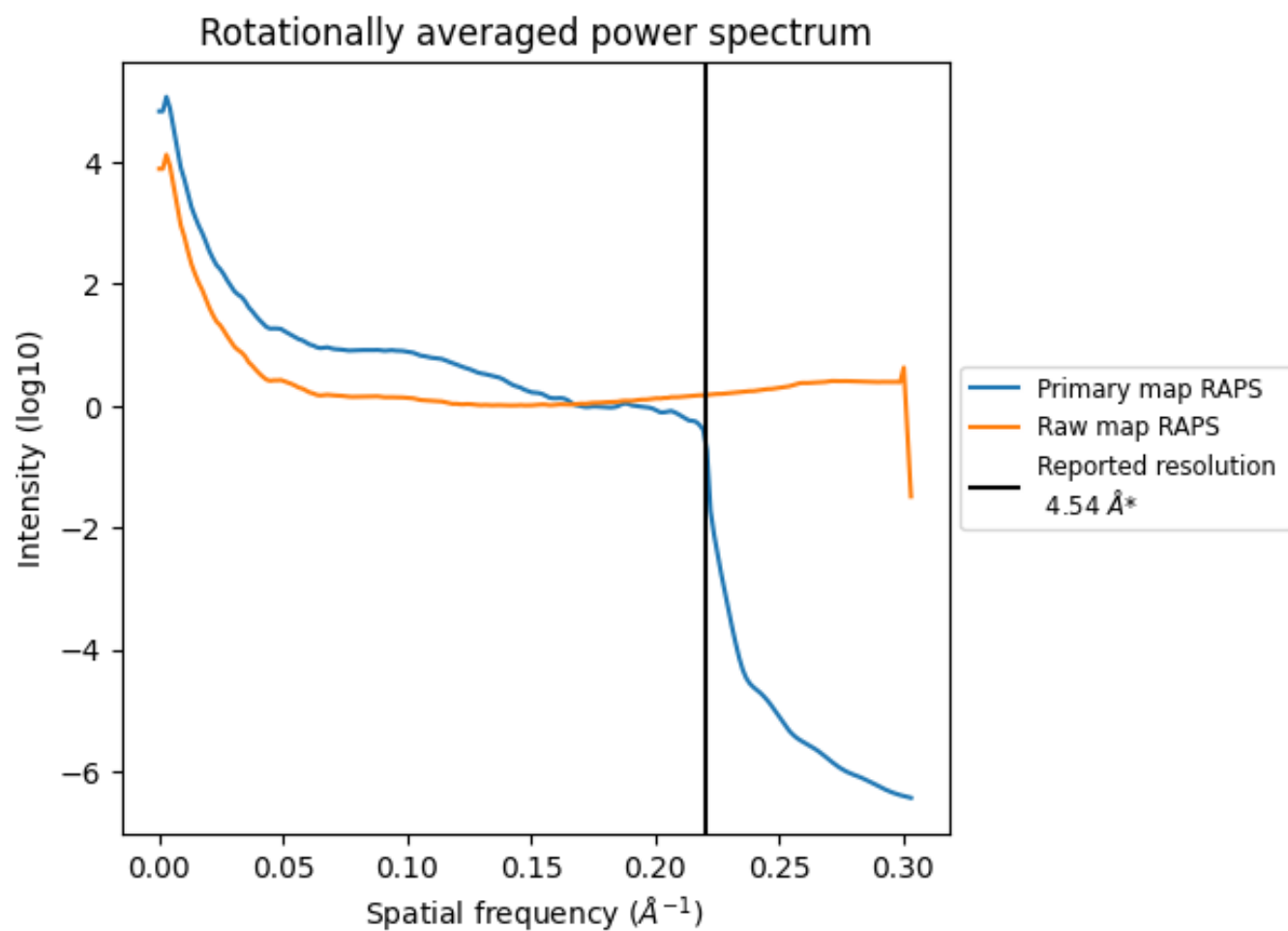
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 724 nm^3 ; this corresponds to an approximate mass of 654 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 ⓘ

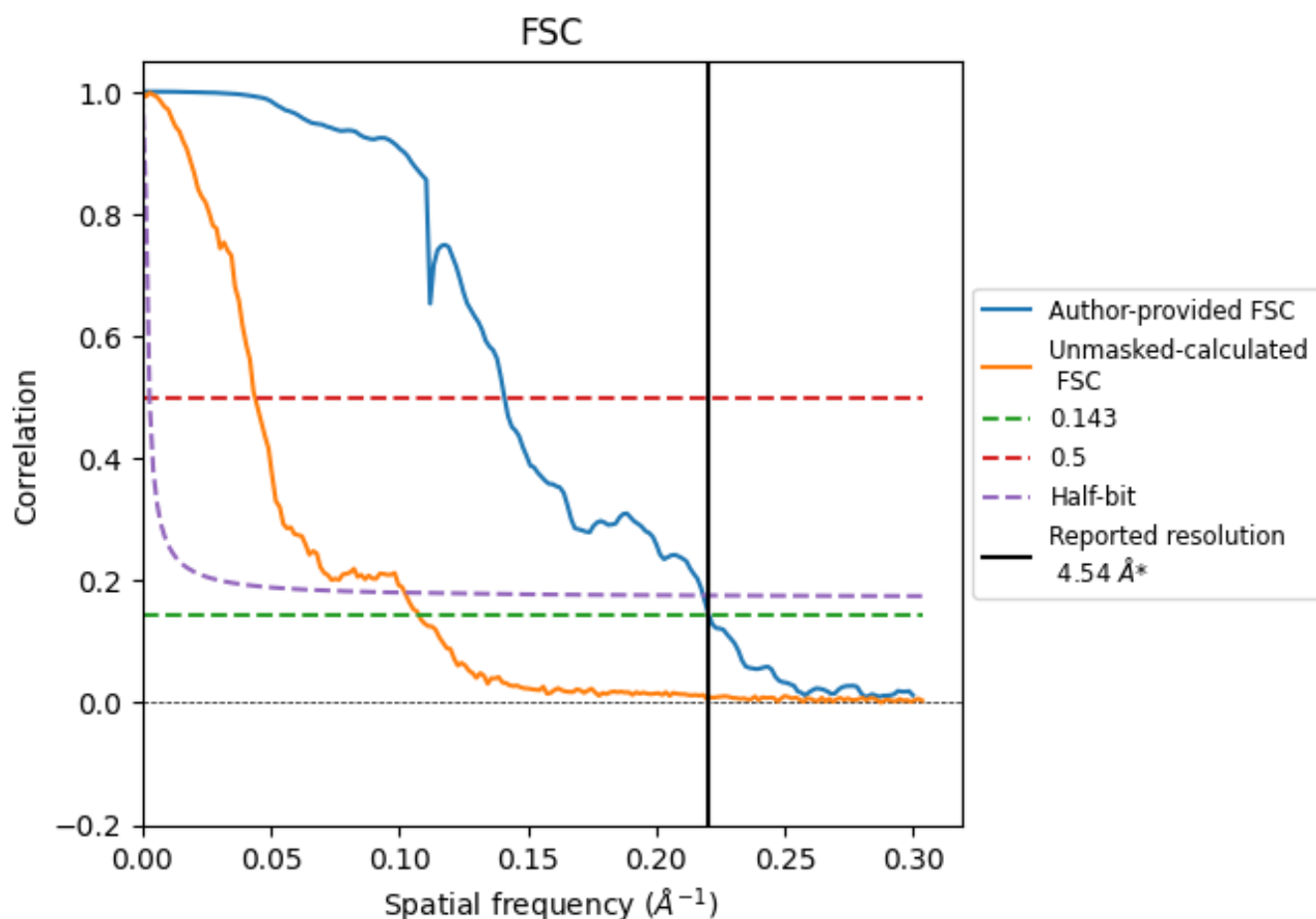


*Reported resolution corresponds to spatial frequency of 0.220 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.220 Å⁻¹

8.2 Resolution estimates [i](#)

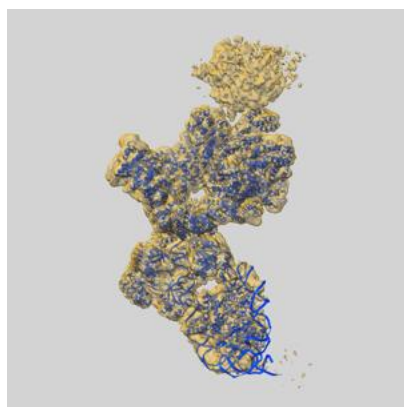
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.54	-	-
Author-provided FSC curve	4.54	7.10	4.58
Unmasked-calculated*	9.29	22.78	9.79

*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 9.29 differs from the reported value 4.54 by more than 10 %

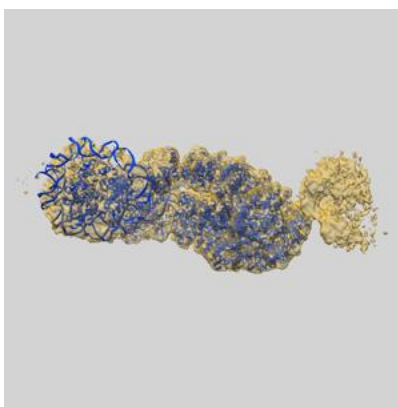
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52958 and PDB model 9Q9F. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

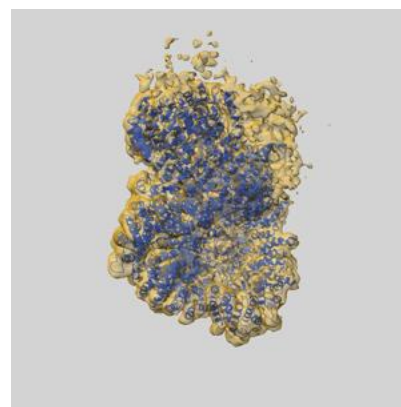
9.1 Map-model overlay [i](#)



X



Y



Z

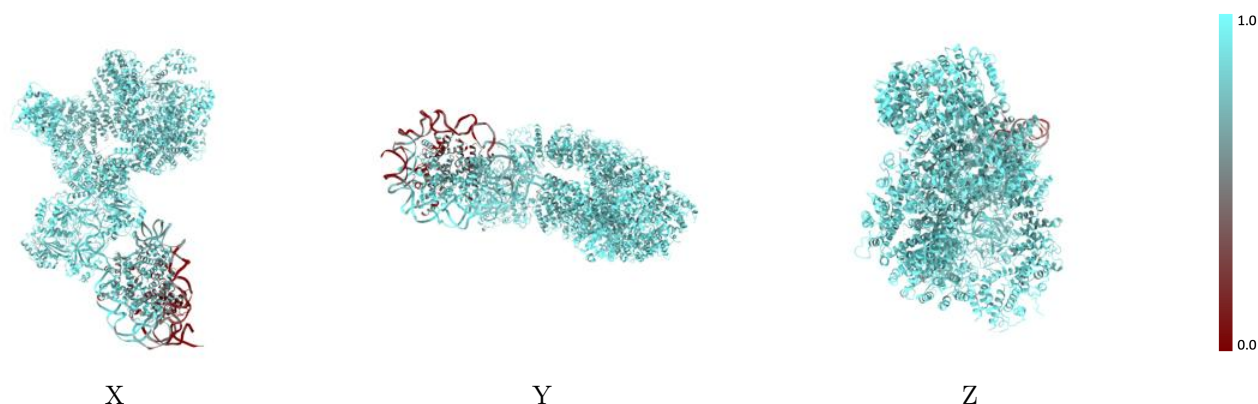
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



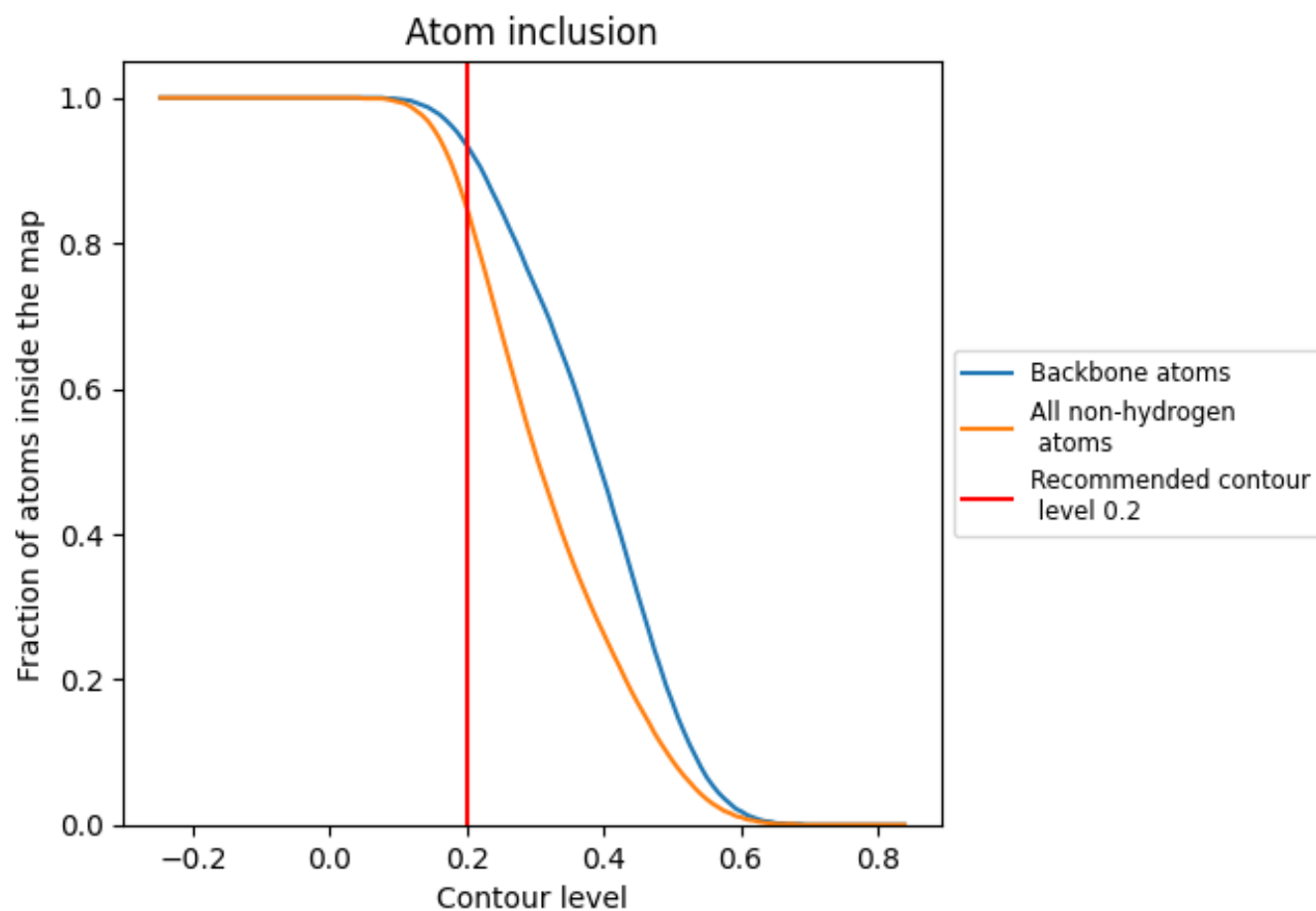
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8500	 0.2150
A	 0.7080	 0.1420
B	 0.8730	 0.1350
C	 0.7110	 0.1680
D	 0.7520	 0.1730
E	 0.4830	 0.1280
F	 0.5730	 0.1700
G	 0.6360	 0.1440
H	 0.6560	 0.1340
I	 0.6720	 0.1590
J	 0.6990	 0.1710
K	 0.9250	 0.2250
L	 0.9060	 0.2030
O	 0.8960	 0.2380

