



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 12:13 AM EDT

PDB ID : 7JGG
EMDB ID : EMD-22326
Title : Cryo-EM structure of P. falciparum VAR2CSA NF45 DBL5 and DBL6 domains at 4.88 Å
Authors : Ma, R.; Tolia, N.H.
Deposited on : 2020-07-19
Resolution : 4.88 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

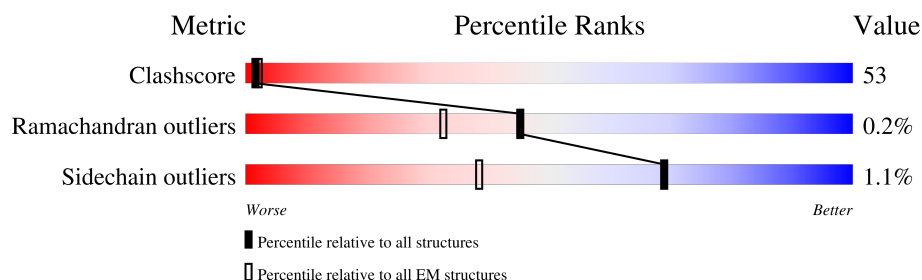
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.88 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	2653	 7% 12% 81%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4210 atoms, of which 28 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 Erythrocyte membrane protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	506	4210	2643	28	713	799	27	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	THR	-	expression tag	UNP W7K270
A	0	GLY	-	expression tag	UNP W7K270
A	2643	GLY	-	expression tag	UNP W7K270
A	2644	THR	-	expression tag	UNP W7K270
A	2645	LYS	-	expression tag	UNP W7K270
A	2646	HIS	-	expression tag	UNP W7K270
A	2647	HIS	-	expression tag	UNP W7K270
A	2648	HIS	-	expression tag	UNP W7K270
A	2649	HIS	-	expression tag	UNP W7K270
A	2650	HIS	-	expression tag	UNP W7K270
A	2651	HIS	-	expression tag	UNP W7K270



VAL	K2566	L2499	I2434	P2369	Q2307	A2238	Q2175	M2106	L2040
LYS	K2567	P2500	I2435	P2370	V2308	I2239	F2176	L2107	C2041
ASN	E2568	N2501	K2436	D2371	D2309	K2244	L2177	T2108	F2042
CYS	Q2569	N2502	D2439	K2372	I2310	K2245	R2178	N2109	S2043
MET	Q2570	D2504	MET	N2374	P2311	Y2246	L2179	I2110	R2044
CYS	S2571	D2505	K2441	L2375	E2315	K2247	I2180	Q2111	I2044
LYS	L2572	E2505	E2442	L2376	ASP	G2248	F2112	F2112	I2045
PRO	N2573	R2510	N2443	F2377	VAL	M2249	K2113	D2113	P2049
PRO	Q2575	W2511	N2444	K2378	ILE	ASP	E2182	D2114	A2050
PRO	Y2576	S2445	S2445	L2379	TYR	GLU	L2185	I2115	A2051
ALA	D2577	E2514	K2448	D2380	ARG	PHE	N2186	K2117	L2052
SER	N2578	W2515	I2449	E2381	LEU	LYS	V2187	R2118	R2053
ASN	N2579	T2516	G2450	LYS	LYS	ASN	C2188	L2119	W2054
ASN	Y2580	E2517	K2451	D2382	HIS	THR	I2189	D2120	L2055
GLY	K2581	N2518	I2384	D2383	HIS	PHE	L2190	R2121	K2056
THR	E2582	F2519	I2452	C2385	GLU	LYS	E2191	L2122	E2057
LYS	T2583	C2520	L2453	K2386	TYR	ASN	E2192	L2123	F2058
HIS	K2584	T2521	G2454	Y2387	ASP	ILE	E2193	E2124	K2059
HIS	A2585	K2522	G2455	K2388	LYS	LYS	H2194	K2125	E2060
HIS	E2586	E2525	G2456	K2389	GLY	GLU	K2195	E2126	E2061
HIS	K2587	L2526	V2457	R2389	N2330	PRO	E2196	T2127	I2062
HIS	E2588	Y2527	G2458	L2393	D2331	ASP	Y2197	N2128	A2066
HIS	E2589	E2528	Q2459	F2394	Y2332	ALA	V2198	N2129	Q2067
HIS	S2590	N2529	N2460	K2395	C2334	ASN	K2199	E2130	S2068
P2591	W2530	W2531	E2461	T2398	N2335	GLU	S2200	E2131	E2069
E2592	W2531	T2532	K2462	Y2399	K2336	PRG	K2201	V2132	G2070
F2594	T2532	T2532	R2463	T2399	Y2337	ALA	S2203	D2134	K2071
K2595	N2535	N2535	K2464	T2399	K2338	ASN	N2204	D2135	F2072
D2596	S2536	S2536	G2465	I2402	N2339	GLU	V2205	W2136	L2073
K2597	A2537	A2537	V2467	I2403	I2340	TYR	T2206	W2137	Y2076
C2598	W2538	W2538	D2468	E2405	N2341	LEU	N2207	E2138	Y2077
N2599	CYS	ASN	M2469	V2406	ASN	LYS	L2208	T2139	N2078
G2600	ASN	ASN	N2470	E2407	MET	HIS	Q2211	N2140	E2079
E2601	THR	THR	K2471	R2408	LYS	CYS	G2209	K2141	
C2602	ASN	ASN	Y2472	L2409	LYS	SER	A2210	K2142	
L2605	G2544	G2544	H2473	K2410	LYS	LYS	E2212	S2143	D2082
E2607	S2545	S2545	I2474	K2411	ASN	LYS	S2213	I2144	K2083
THR	V2546	V2546	W2475	V2412	ASN	CYS	E2214	W2145	E2084
LYS	D2547	D2547	E2476	Y2413	ASP	PRO	S2215	K2153	K2085
ASP	K2548	K2548	M2478	E2415	THR	GLY	K2216	K2154	A2086
GLU	N2549	N2549	L2479	A2416	TRP	PHE	C2218	E2088	L2087
THR	E2550	E2550	K2483	K2417	THR	ASN	T2219	K2158	K2089
ARG	C2551	C2551	Y2486	T2418	D2354	ASP	I2222	I2159	K2090
TRP	E2553	E2553	G2487	K2419	L2355	MET	K2223	I2160	K2091
ASN	K2556	K2556	ASN	V2420	K2357	GLN	K2224	D2161	N2092
PRO	N2557	N2557	ILE	K2425	N2358	ILE	Y2225	P2162	S2093
TYR	W2558	W2558	SER	Y2426	S2359	THR	Q2226	F2094	F2094
GLU	Y2559	Y2559	GLU	F2427	S2360	LYS	E2227	Y2095	Y2095
THR	N2560	N2560	ASN	A2429	D2361	LYS	W2228	C2165	I2097
LEU	F2561	F2561	ARG	D2430	ILE	TYR	T2229	T2166	S2096
ASP	I2562	I2562	LYS	I2431	ASN	ASN	R2230	I2167	E2098
THR	L2563	L2563	MET	G2432	LYS	LYS	K2231	P2168	Y2099
GLU	K2564	K2564	L2497	S2433	G2365	K2302	R2232	T2169	I2101
			D2498		V2366	Q2303	W2236	T2172	K2102
					L2367	I2304	E2237	P2173	G2103
						K2305		S2104	P2105

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157702	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 ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	29.549	Depositor
Minimum map value	-4.473	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size (\AA)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.058, 1.058, 1.058	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	0.24	0/4264	0.38	1/5710 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	2040	LEU	CB-CG-CD1	5.92	121.06	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2039	GLN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4182	28	4095	440	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4182	28	4095	440	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 53.

The worst 5 of 440 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)
1:A:2548:LYS:HE3	1:A:2550:GLU:HB3	1.38	1.04
1:A:2244:LYS:HG2	1:A:2247:LYS:HE2	1.37	1.03
1:A:2198:VAL:HG21	1:A:2222:ILE:HD13	1.42	1.01
1:A:2369:PRO:HG2	1:A:2372:ARG:HB3	1.44	0.98
1:A:2407:GLU:HA	1:A:2410:LYS:HZ3	1.27	0.98

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	490/2653 (18%)	473 (96%)	16 (3%)	1 (0%)	44 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2040	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	461/2419 (19%)	456 (99%)	5 (1%)	70 80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2191	LYS
1	A	2336	LYS
1	A	2372	ARG
1	A	2419	LYS
1	A	2465	LYS

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

Mol	Chain	Res	Type
1	A	2140	ASN
1	A	2175	GLN
1	A	2374	ASN
1	A	2459	GLN
1	A	2506	HIS

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

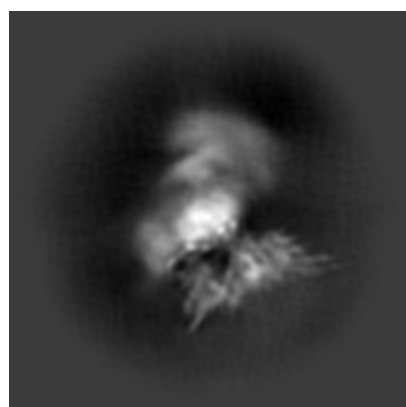
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22326. These allow visual inspection of the internal detail of the map and identification of artifacts.

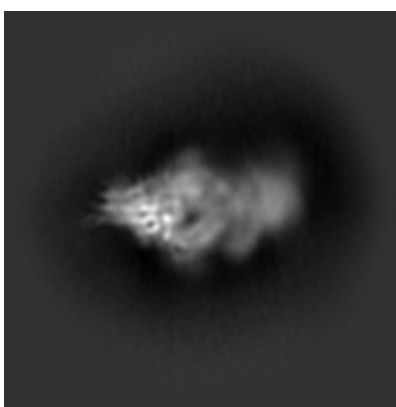
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

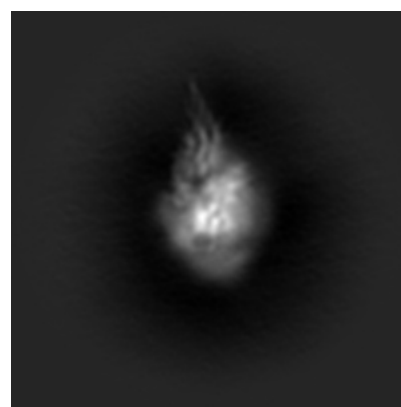
6.1.1 Primary map



X



Y

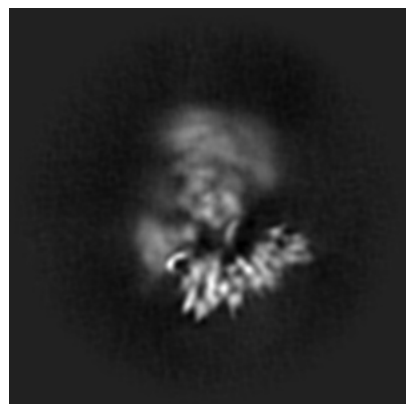


Z

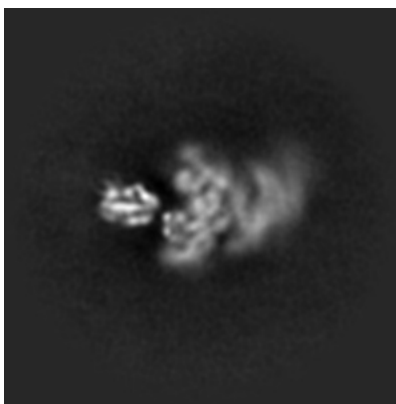
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

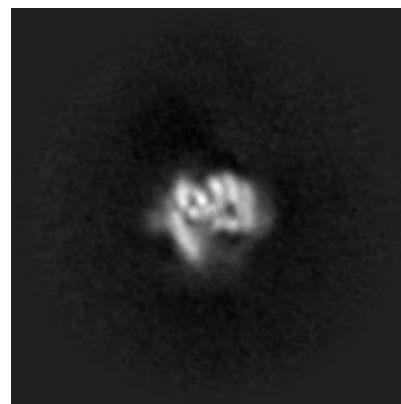
6.2.1 Primary map



X Index: 150



Y Index: 150

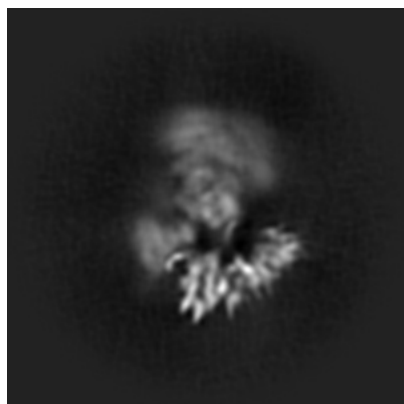


Z Index: 150

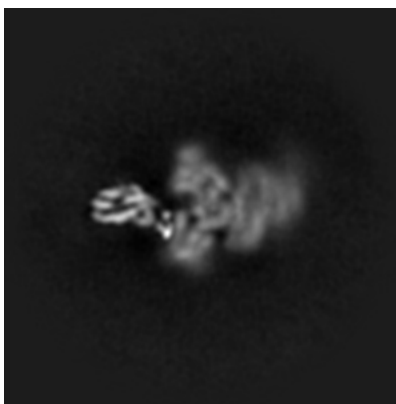
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

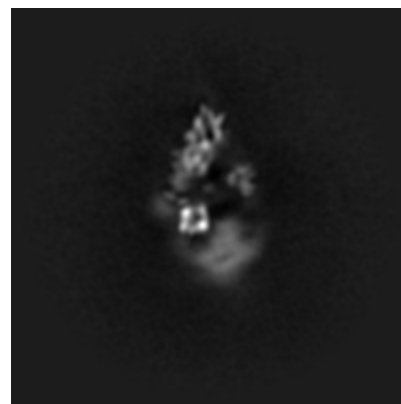
6.3.1 Primary map



X Index: 152



Y Index: 144

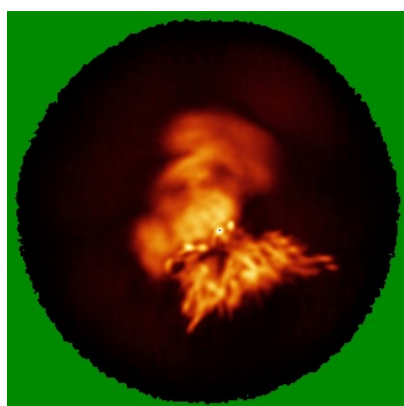


Z Index: 122

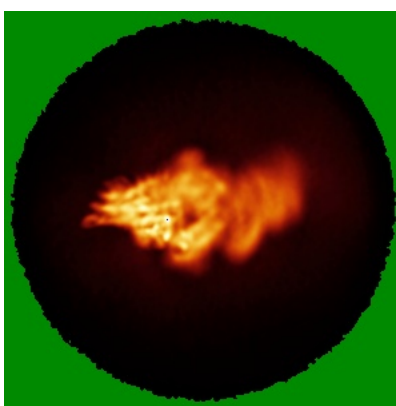
The images above show the largest variance slices of the map in three orthogonal directions.

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

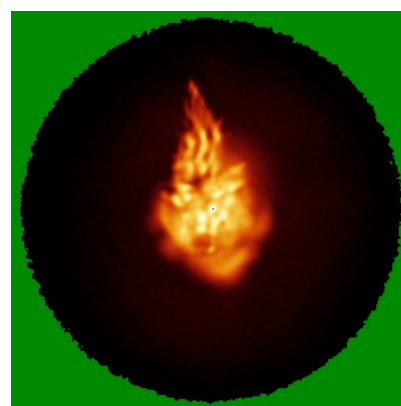
6.4.1 Primary map



X



Y

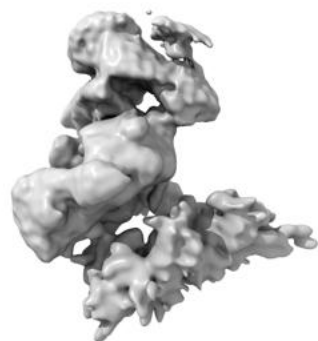


Z

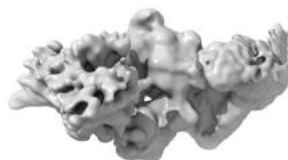
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

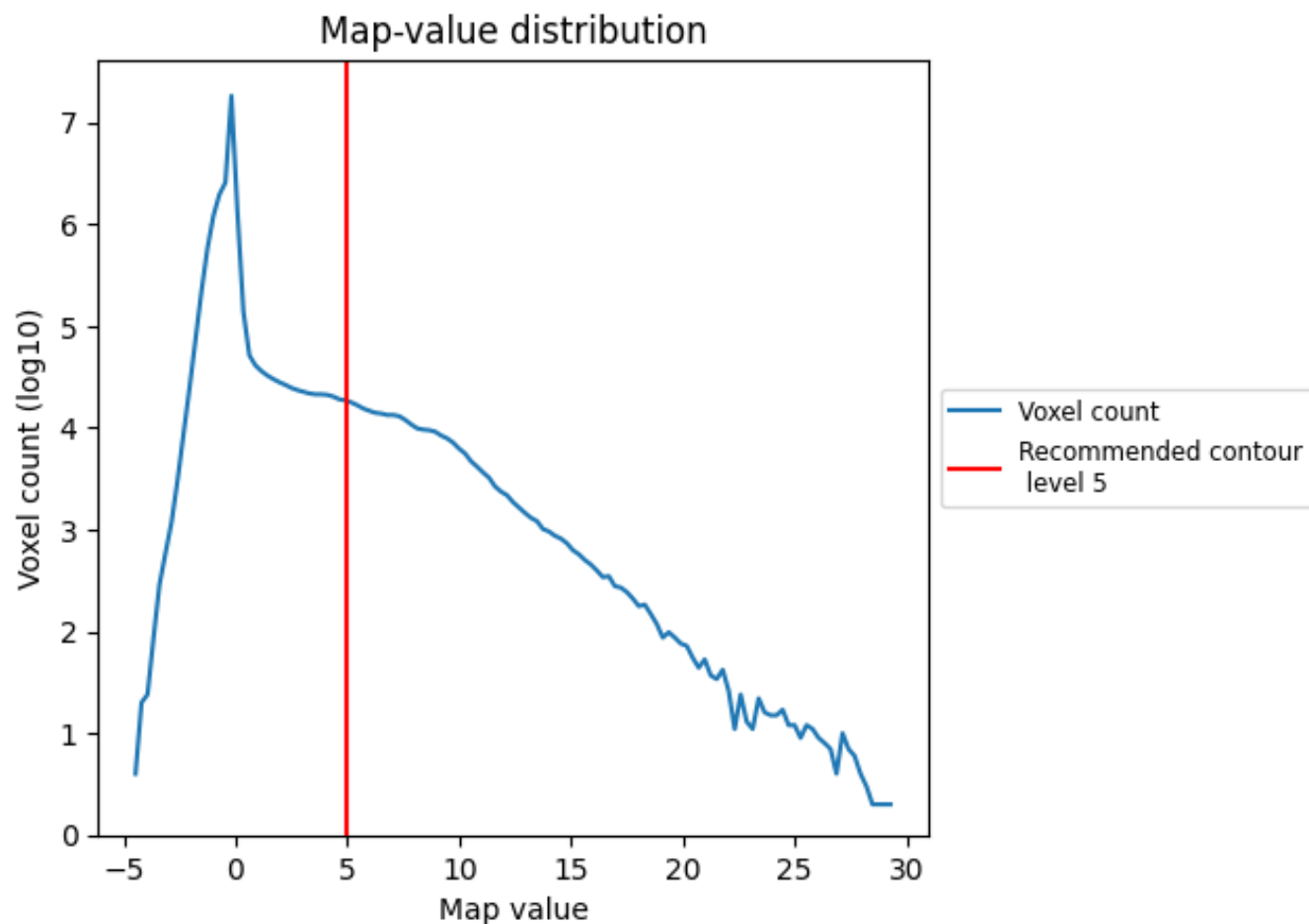
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

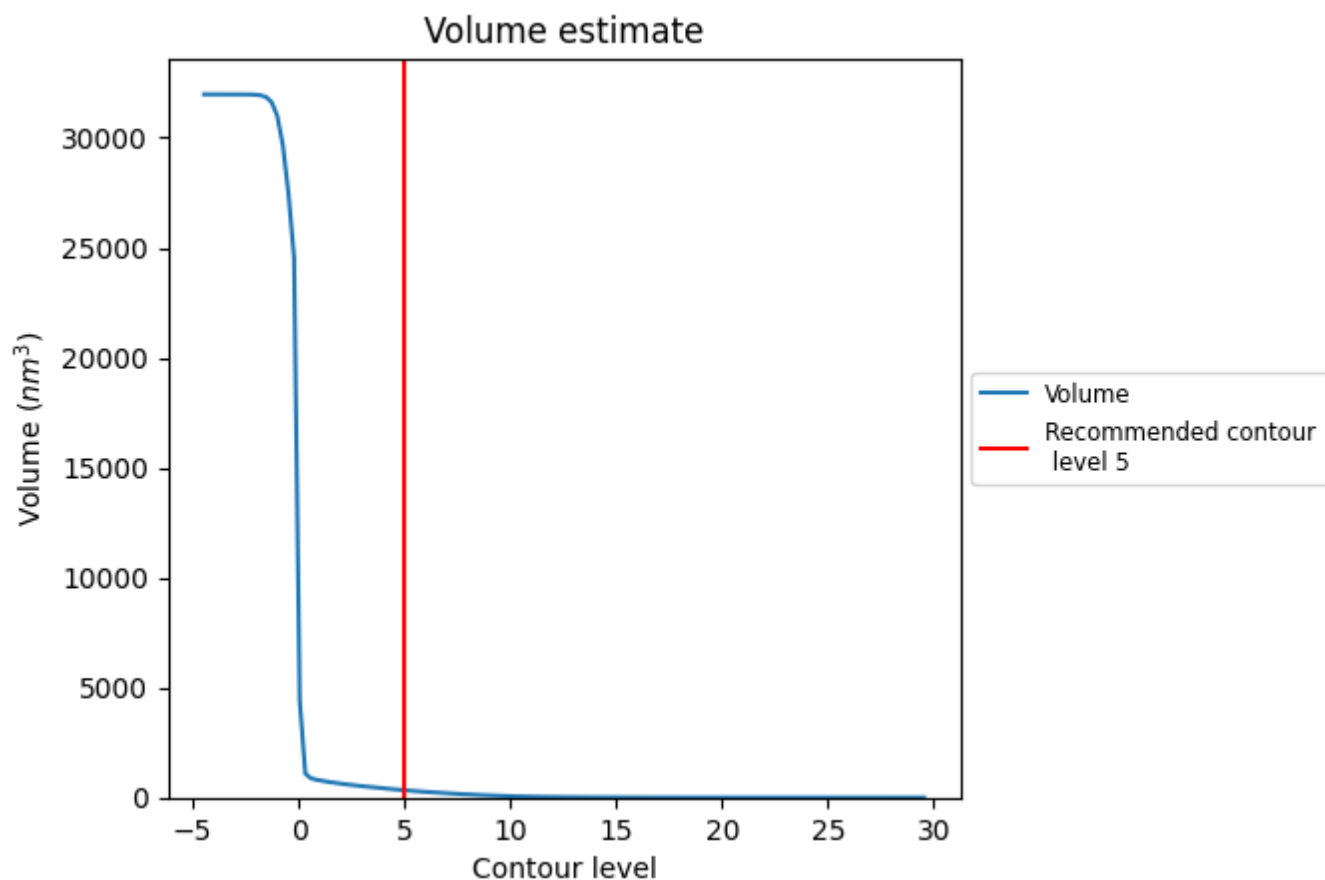
This section contains the results of statistical analysis of the map.

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.

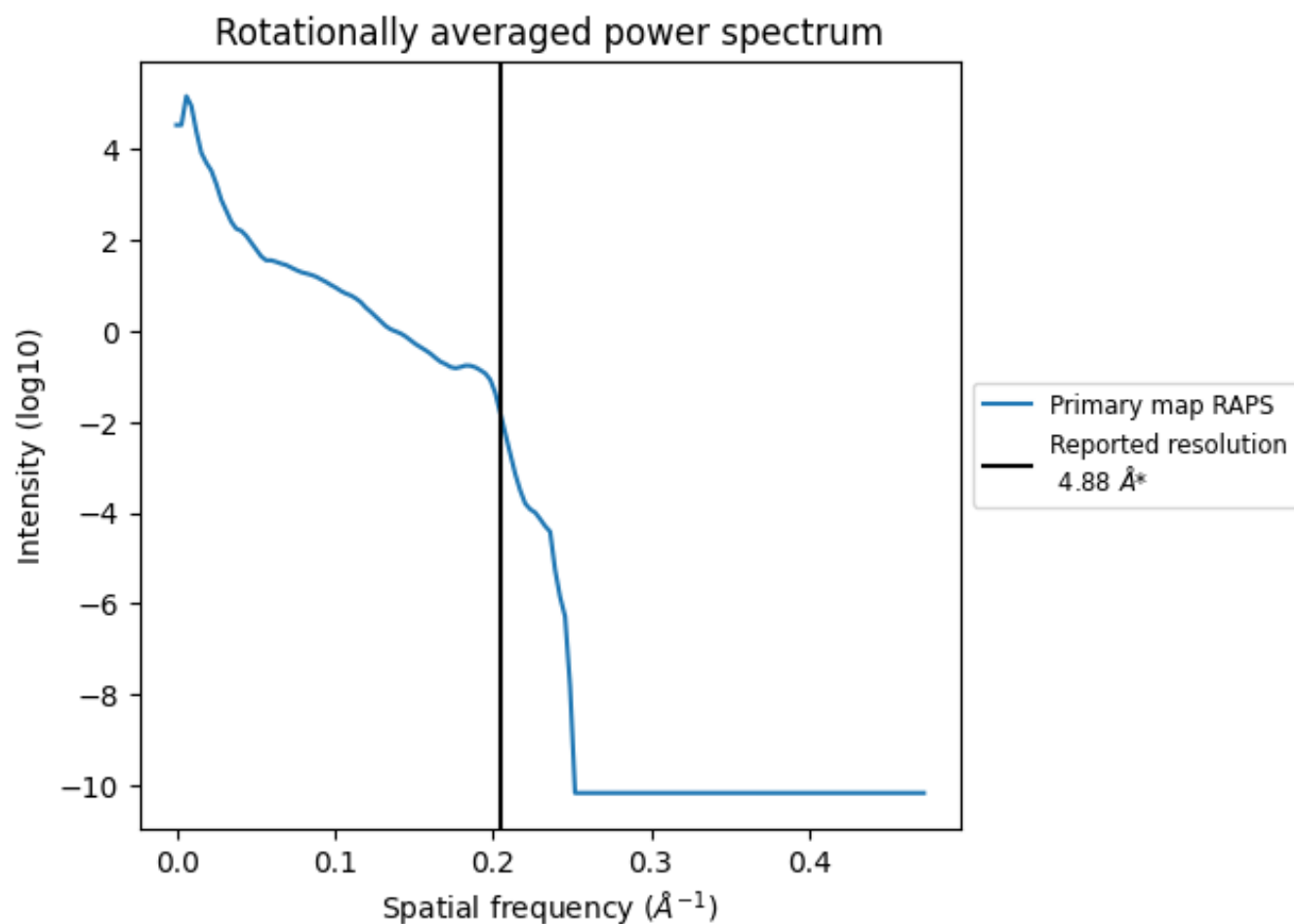
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332 nm^3 ; this corresponds to an approximate mass of 300 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 0.205 Å⁻¹

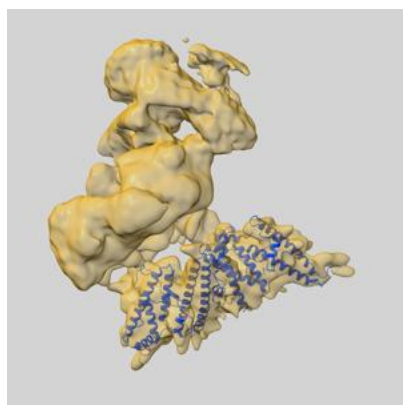
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

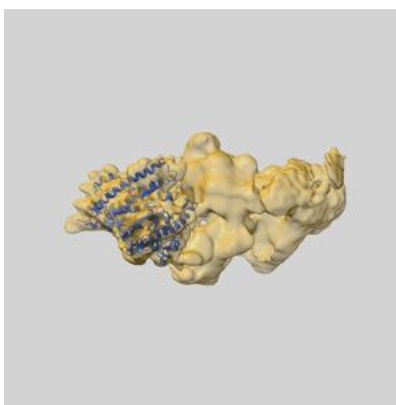
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22326 and PDB model 7JGG. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

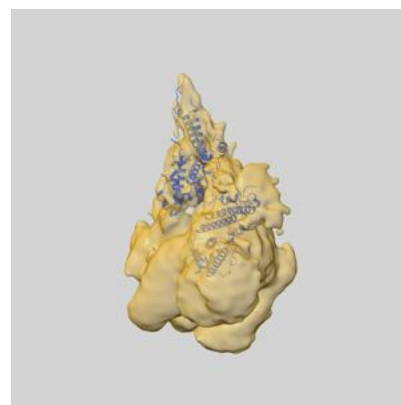
9.1 Map-model overlay [i](#)



X



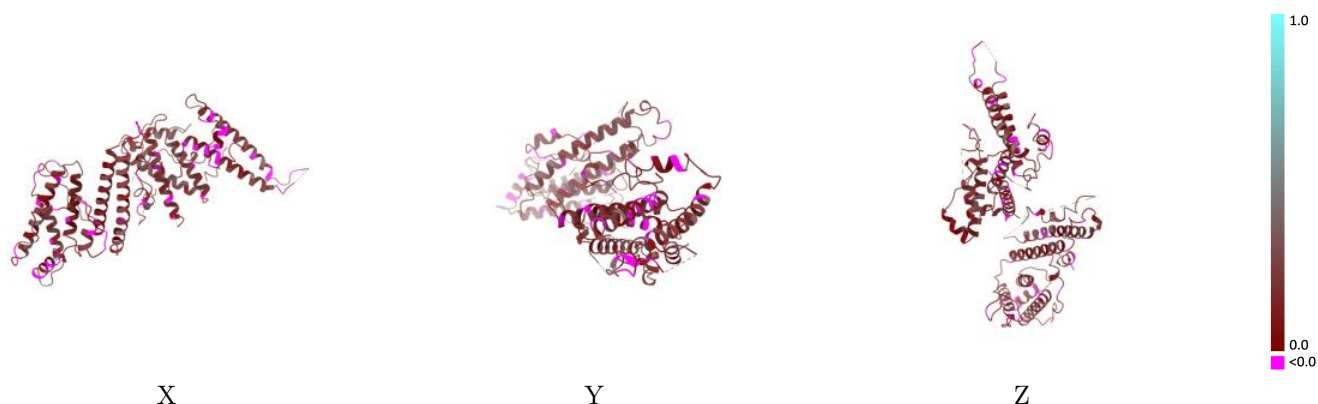
Y



Z

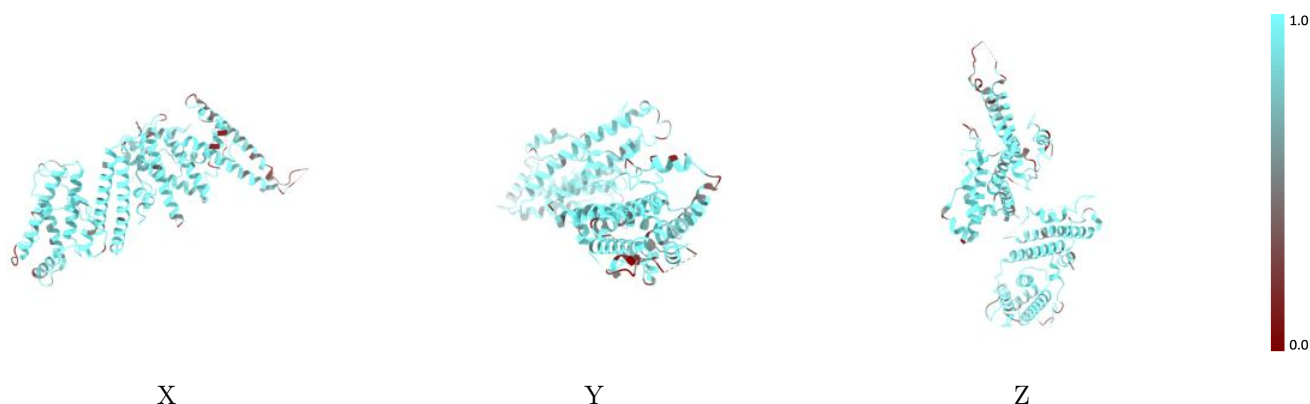
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



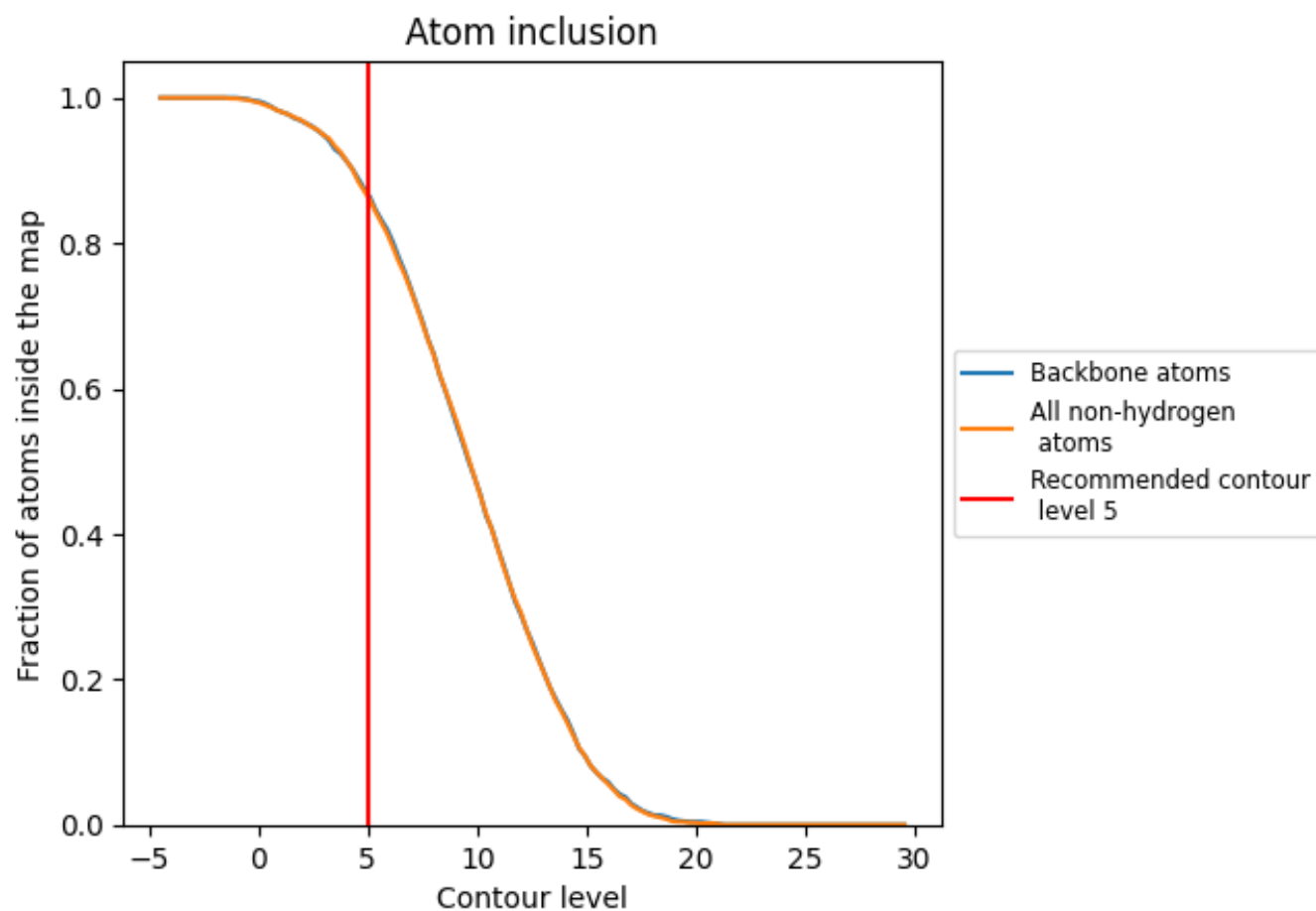
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% 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 (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8640	<div><div></div></div> 0.1540
A	<div><div></div></div> 0.8660	<div><div></div></div> 0.1540

