



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 03:26 AM EST

PDB ID : 7JGF
EMDB ID : EMD-22325
Title : Cryo-EM structure of P. falciparum VAR2CSA FCR3 domains DBL5 and DBL6 at 4.69 Å
Authors : Ma, R.; Tolia, N.H.
Deposited on : 2020-07-19
Resolution : 4.69 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

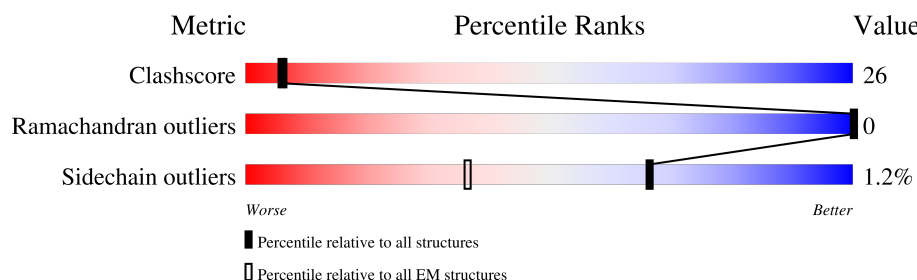
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.69 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	2660	<div> <div>12%</div> <div>10% 10% 80%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4477 atoms, of which 30 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	532	4477	2808	30	770	839	30	4	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	THR	-	expression tag	UNP Q6UDW7
A	0	GLY	-	expression tag	UNP Q6UDW7
A	2650	GLY	-	expression tag	UNP Q6UDW7
A	2651	THR	-	expression tag	UNP Q6UDW7
A	2652	LYS	-	expression tag	UNP Q6UDW7
A	2653	HIS	-	expression tag	UNP Q6UDW7
A	2654	HIS	-	expression tag	UNP Q6UDW7
A	2655	HIS	-	expression tag	UNP Q6UDW7
A	2656	HIS	-	expression tag	UNP Q6UDW7
A	2657	HIS	-	expression tag	UNP Q6UDW7
A	2658	HIS	-	expression tag	UNP Q6UDW7



HIS	S2543	R2481	A2421	I2360	F2298	R2236	S2169	D2105	I2039
ILE	K2544	E2482	M2422	S2361	K2299	K2237	W2170	I2106	P2040
ASP	C2545	A2483	K2423	N2362	Q2300	R2238	C2171	I2107	P2041
LYS	T2546	E2484	Y2424	G2363	I2301	S2239	I2172	K2108	R2042
ASN	H2547	G2485	S2425	V2364	K2302	I2240	I2173	D2111	R2043
LYS	A2548	D2486	F2426	L2365	E2303	R2241	P2179	M2112	R2044
THR	C2549	T2487	T2427	I2366	Q2304	W2242	P2180	L2113	Q2045
TRP	V2550	E2488	D2428	F2367	V2305	E2243	Q2181	T2114	L2046
ASN	N2551	T2489	I2429	R2368	K2306	E2244	P2182	N2115	C2047
PRO	Y2552	N2490	G2430	R2369	I2307	I2245	L2183	I2116	F2048
LYS	N2553	E2491	I2432	K2370	E2310	S2246	R2184	E2117	R2050
THR	Y2555	N2492	I2433	K2371	L2311	K2247	W2185	F2118	I2051
GLU	L2557	R2494	K2434	W2372	E2312	R2248	I2186	K2119	
ASP	T2558	F2495	G2435	L2373	ASP	Y2249	I2187	K2120	P2055
THR	W2559	T2496	D2437	F2374	VAL	K2250	K2187	D2120	A2056
PHE	K2560	D2497	D2438	L2375	ILE	K2251	E2188	I2121	A2057
LYS	T2561	M2438	M2439	D2378	ARG	Y2252	W2189	I2123	L2058
SER	E2562	E2440	E2440	P2379	ILE	K2254	Q2190	K2124	
CYS	Y2563	K2441	M2439	S2380	LYS	W2255	T2191	L2125	I2061
ASP	E2564	N2442	E2441	K2381	HIS	D2256	N2192	L2126	N2062
CYS	T2565	S2443	K2442	I2382	GLU	Y2257	C2194	R2127	E2063
PRO	Q2566	S2443	S2443	C2383	TYR	L2258	I2195	L2128	F2064
LYS	T2567	S2444	S2444	E2384	ASP	K2259	Q2196	L2129	K2065
PRO	N2568	D2445	D2445	Y2385	LYS	D2260	K2197	E2130	E2066
LEU	K2569	K2446	K2446	K2386	GLY	W2261	Q2198	E2130	E2067
SER	T2570	I2447	I2447	K2387	N2327	K2262	Q2199	T2133	I2069
PRO	D2571	G2448	G2448	D2388	D2328	E2263	H2200	N2134	L2070
ILE	N2572	K2449	K2449	P2389	Y2329	PR0	K2201	N2135	K2071
LYS	Q2509	I2450	I2450	K2390	I2330	ASP	E2202	T2136	A2072
ASP	E2510	L2451	L2451	N2332	C2331	ALA	Y2203	K2137	Q2073
ASP	W2511	G2452	G2452	K2333	K2333	ASN	V2204	K2138	S2074
LEU	S2512	D2453	D2453	Y2392	THR	THR	K2205	A2139	K2077
PRO	E2513	T2454	T2454	K2393	TYR	TYR	S2206	E2140	F2078
PRO	N2514	G2455	G2455	F2394	LEU	LEU	K2207	D2141	L2079
ALA	F2515	D2456	D2456	F2395	ARG	ARG	C2208	W2142	L2079
ASP	C2516	G2457	G2457	I2396	GLU	GLU	S2209	W2143	Q2080
GLU	D2517	Q2457	Q2457	T2397	HIS	HIS	N2210	K2144	N2081
PRO	R2518	N2458	N2458	W2398	CYS	CYS	T2145	T2145	Y2082
PRO	R2519	E2459	E2459	S2399	SER	SER	N2211	N2146	Y2083
GLY	Q2520	K2460	K2460	A2400	MET	MET	T2212	K2147	K2084
THR	K2521	K2461	K2461	F2401	LYS	LYS	T2213	K2148	E2085
LYS	L2522	K2462	K2462	T2402	ASN	ASN	N2214	S2149	H2086
HIS	Y2523	K2463	K2463	E2403	GLY	GLY	L2214	T2150	K2087
HIS	D2524	W2464	W2464	V2404	PHE	PHE	Q2215	W2151	I2088
HIS	K2525	W2465	W2465	E2405	ASP	ASP	A2216	N2152	I2088
HIS	L2526	D2466	D2466	K2406	ASN	ASN	Q2217	A2153	K2089
LYS	N2527	M2467	M2467	L2407	PHE	PHE	A2218	N2154	E2090
LYS	S2528	K2468	K2468	K2408	V2349	MET	A2219	K2091	K2091
LYS	E2529	N2468	N2468	K2409	T2350	GLU	S2219	A2092	A2092
LYS	C2530	K2469	K2469	A2410	MET	MET	N2223	G2157	L2093
LYS	I2531	Y2470	Y2470	Y2411	ASN	ASN	C2224	Y2158	E2094
LYS	I2532	H2471	H2471	G2412	ASN	ASN	T2225	K2160	A2095
LYS	W2473	I2472	I2472	G2413	K2356	K2295	I2228	N2163	F2100
LYS	A2533	E2474	E2474	K2414	S2357	E2296	K2229	K2164	Y2101
LYS	E2534	S2475	S2475	K2415	N2358	A2297	Y2231	I2165	D2102
LYS	C2535	N2476	N2476	A2416	E2359		Q2232	I2166	Y2103
LYS	T2536	L2477	L2477	K2417			E2233	D2167	E2104
LYS	C2539	G2478	G2478	Y2418			W2234	P2168	
LYS	V2540	Y2480	Y2480	H2420			S2235		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	271442	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 ($e^-/\text{\AA}^2$)	71.2	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	49.984	Depositor
Minimum map value	-20.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	6.73	Depositor
Map size (Å)	270.848, 270.848, 270.848	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.25	0/4564	0.43	0/6120

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	A	4447	30	4371	230	0
All	All	4447	30	4371	230	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 26.

The worst 5 of 230 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:2072:ALA:HB1	1:A:2150:ILE:HD12	1.41	1.01
1:A:2373:LEU:HD22	1:A:2432:ILE:HD13	1.51	0.92
1:A:2165:ILE:HG13	1:A:2173:ILE:HG22	1.49	0.92
1:A:2502:PRO:HD2	1:A:2505:LEU:HD22	1.53	0.91
1:A:2233:GLU:HG3	1:A:2237:LYS:HE2	1.55	0.88

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	529/2660 (20%)	505 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	493/2412 (20%)	486 (99%)	7 (1%)	62	76

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

Mol	Chain	Res	Type
1	A	2417	LYS
1	A	2463	LYS
1	A	2518[B]	ARG
1	A	2518[A]	ARG
1	A	2370	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2135	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

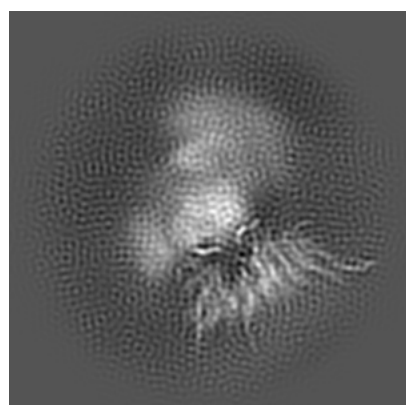
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22325. These allow visual inspection of the internal detail of the map and identification of artifacts.

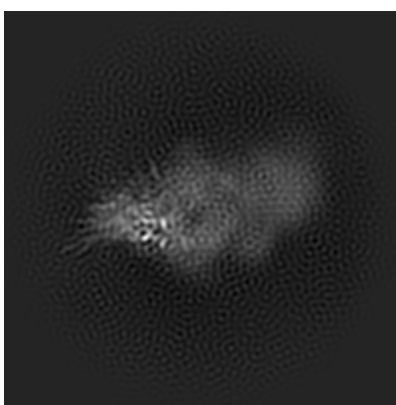
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

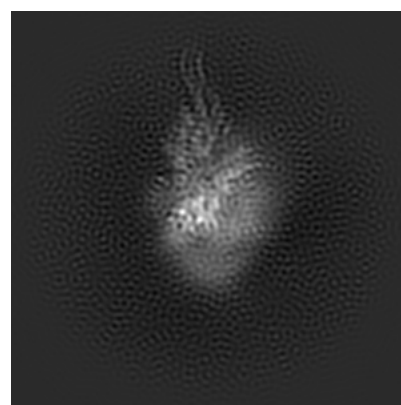
6.1.1 Primary map



X



Y

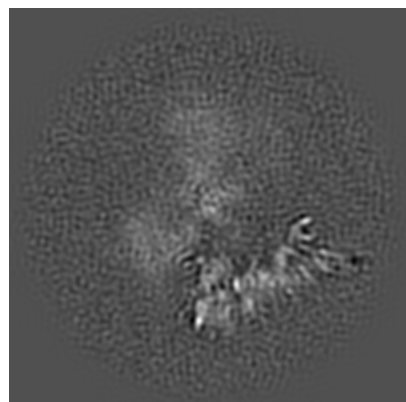


Z

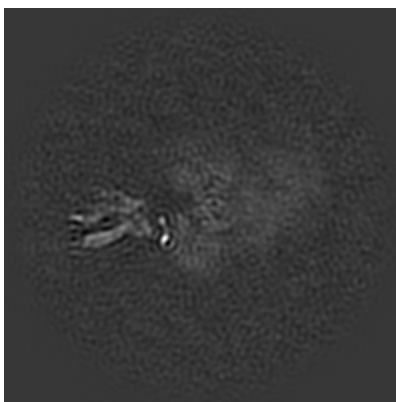
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

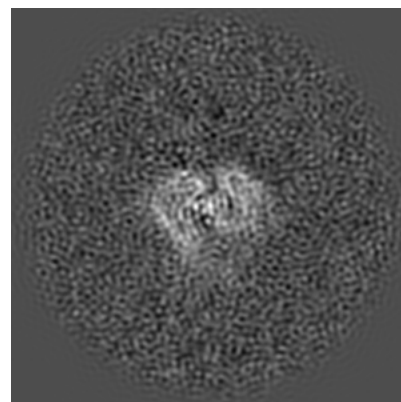
6.2.1 Primary map



X Index: 128



Y Index: 128

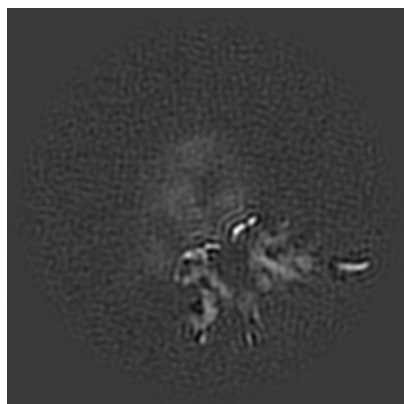


Z Index: 128

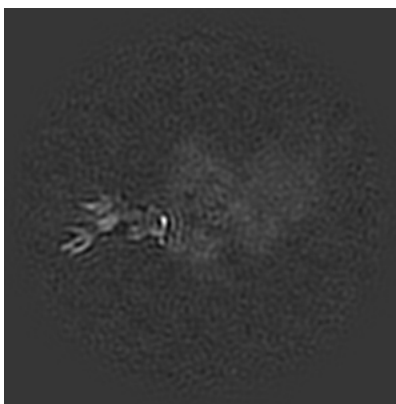
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

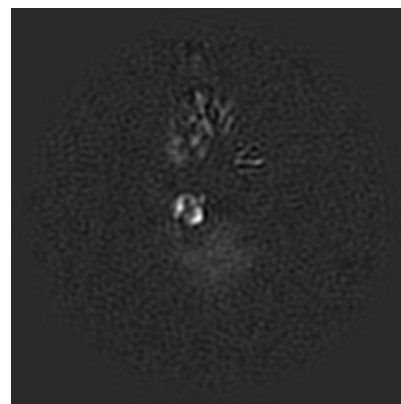
6.3.1 Primary map



X Index: 110



Y Index: 121

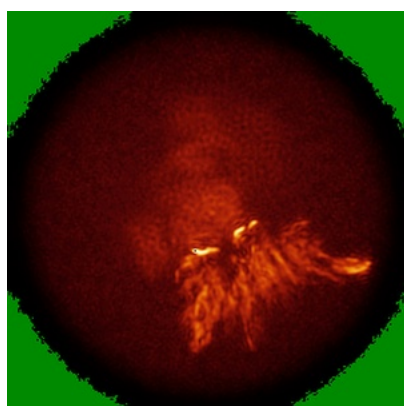


Z Index: 102

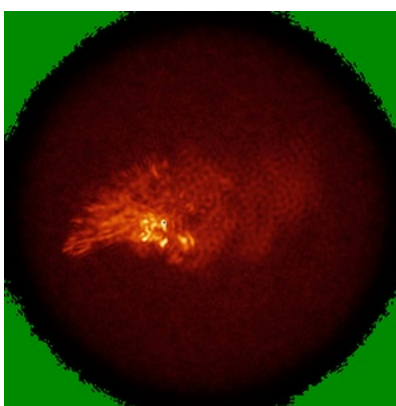
The images above show the largest variance slices of the map in three orthogonal directions.

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

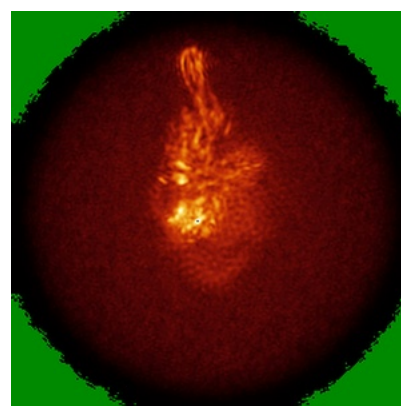
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 6.73. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

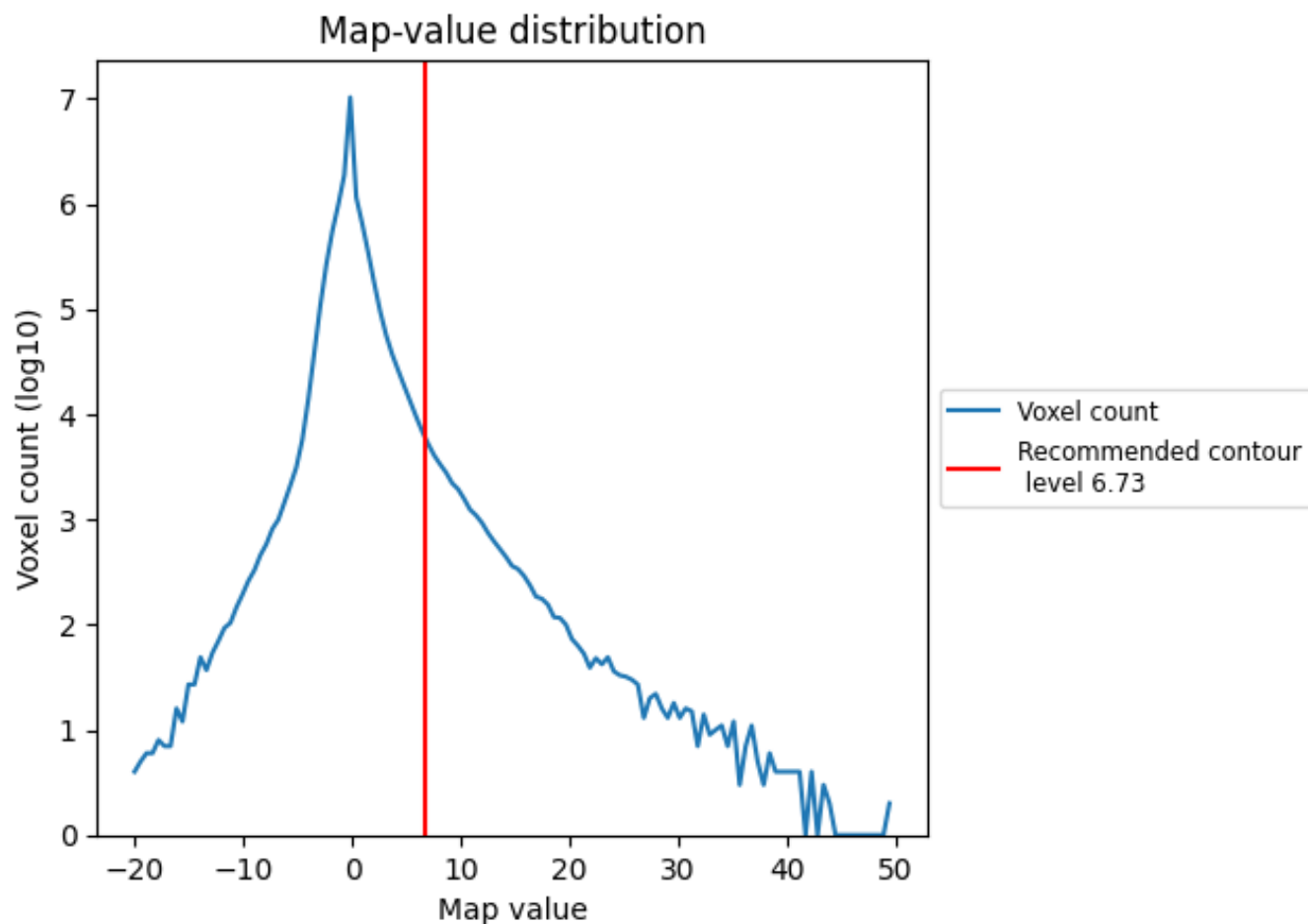
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

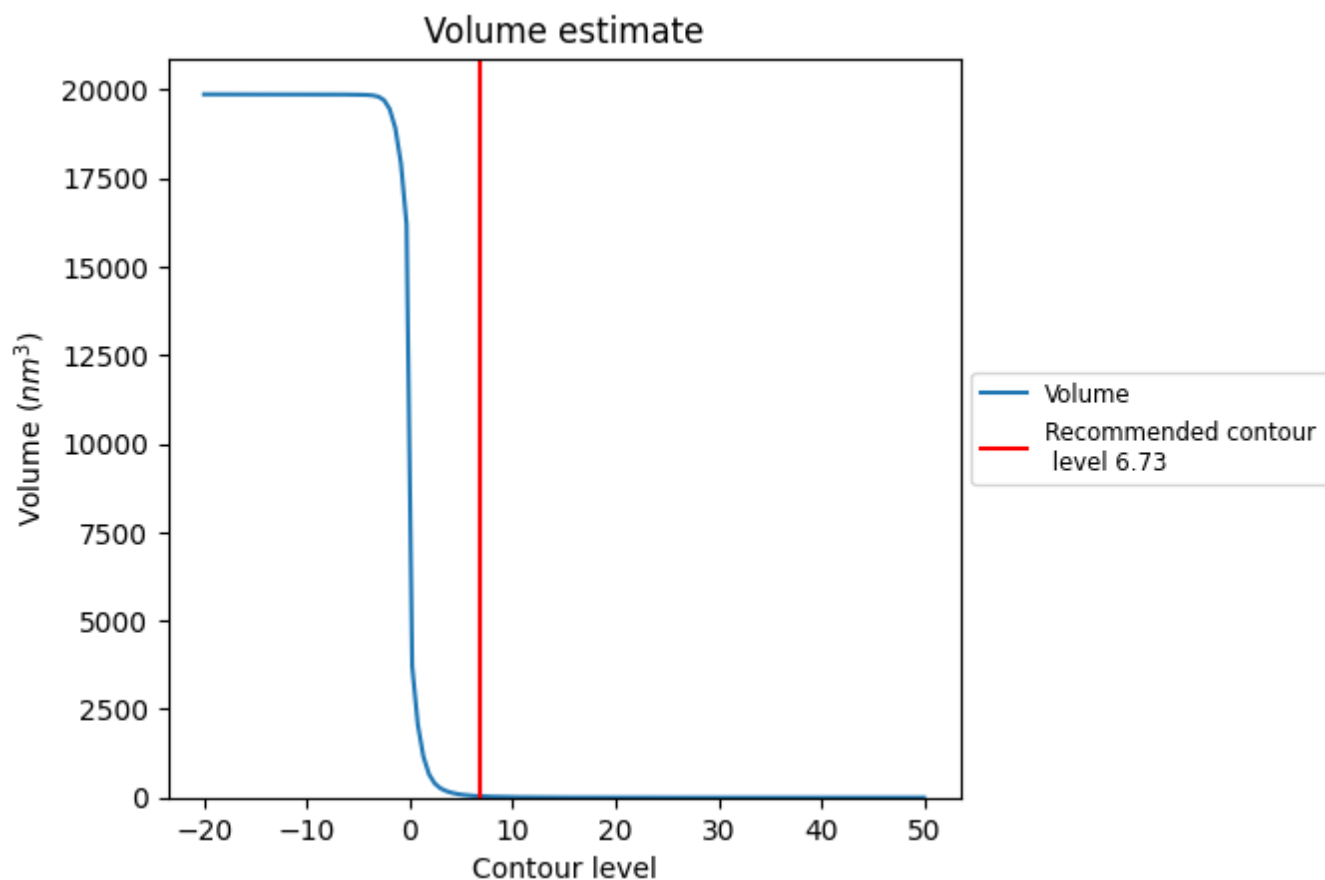
This section contains the results of statistical analysis of the map.

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.

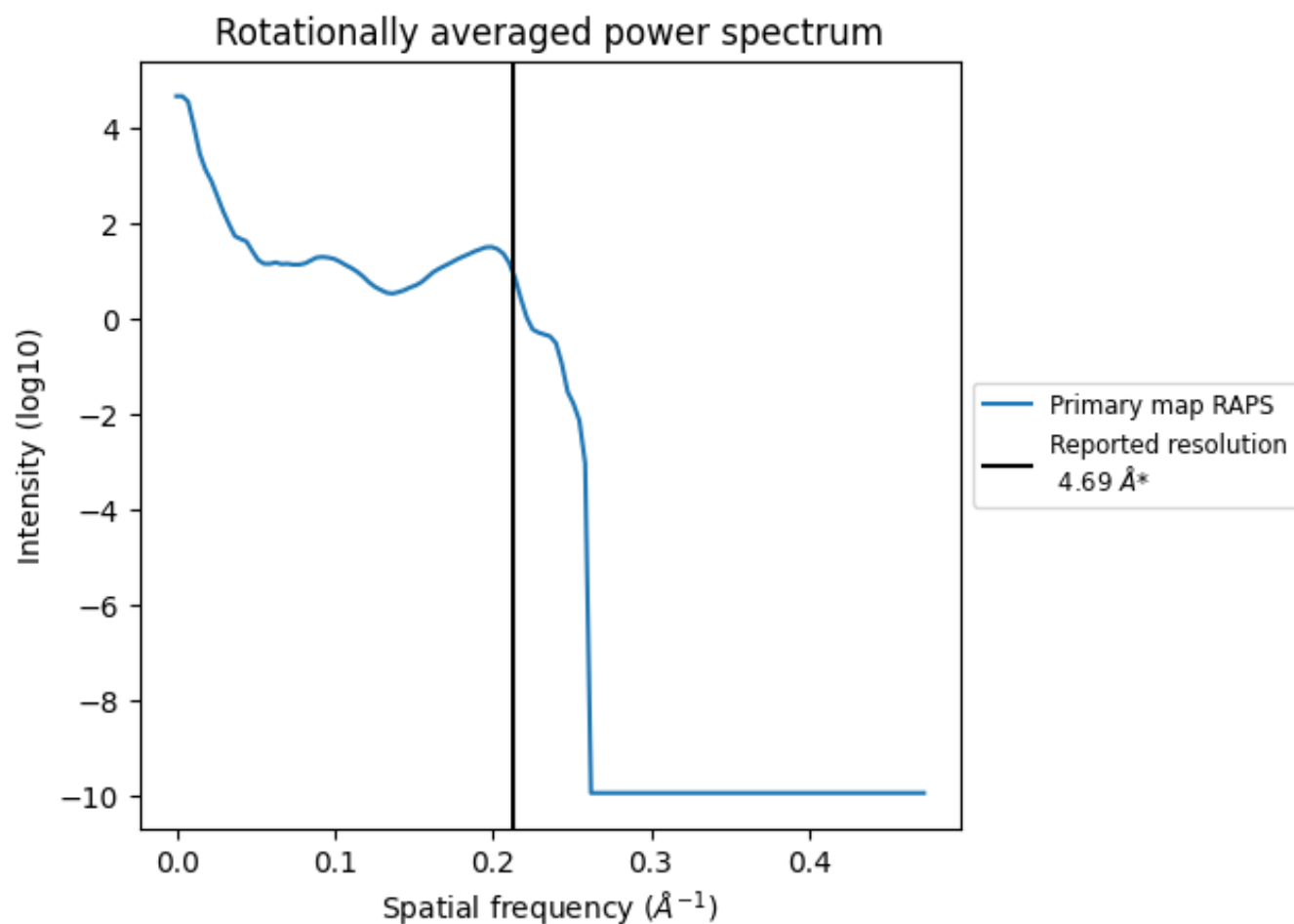
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm^3 ; this corresponds to an approximate mass of 35 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 0.213 Å⁻¹

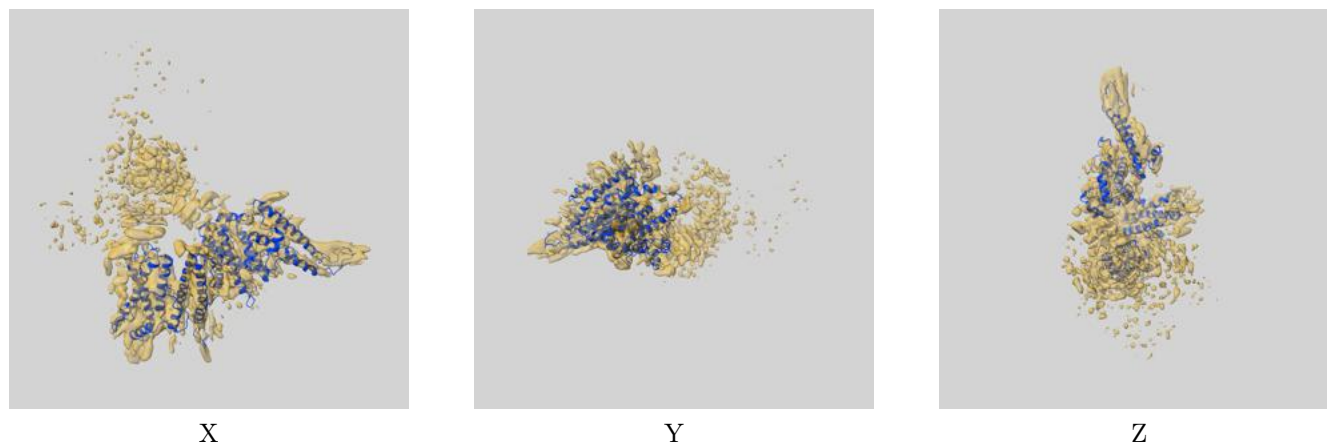
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

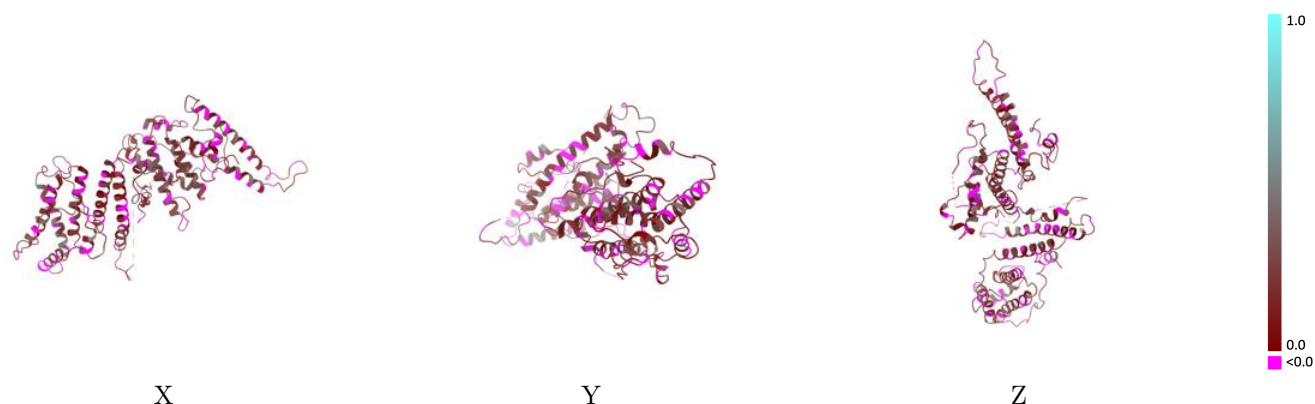
This section contains information regarding the fit between EMDB map EMD-22325 and PDB model 7JGF. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



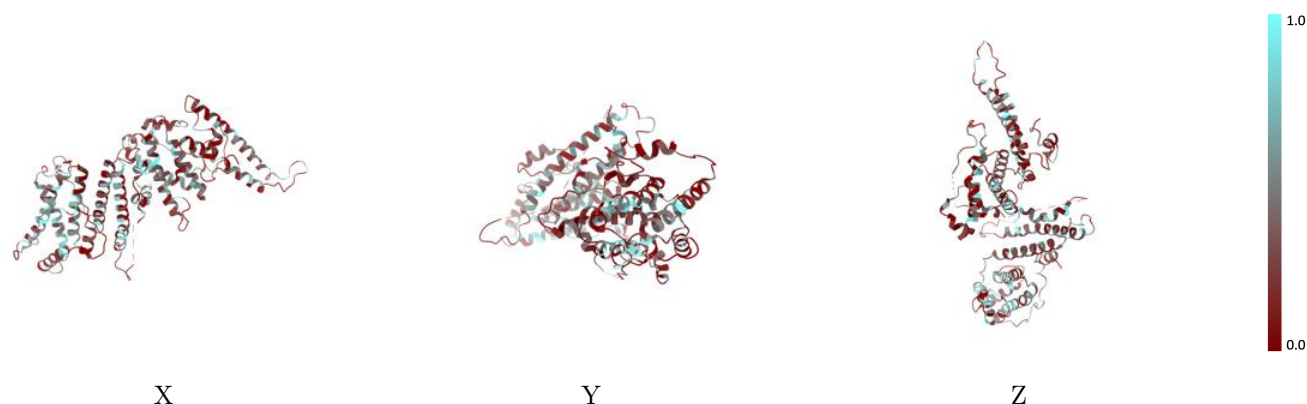
The images above show the 3D surface view of the map at the recommended contour level 6.73 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



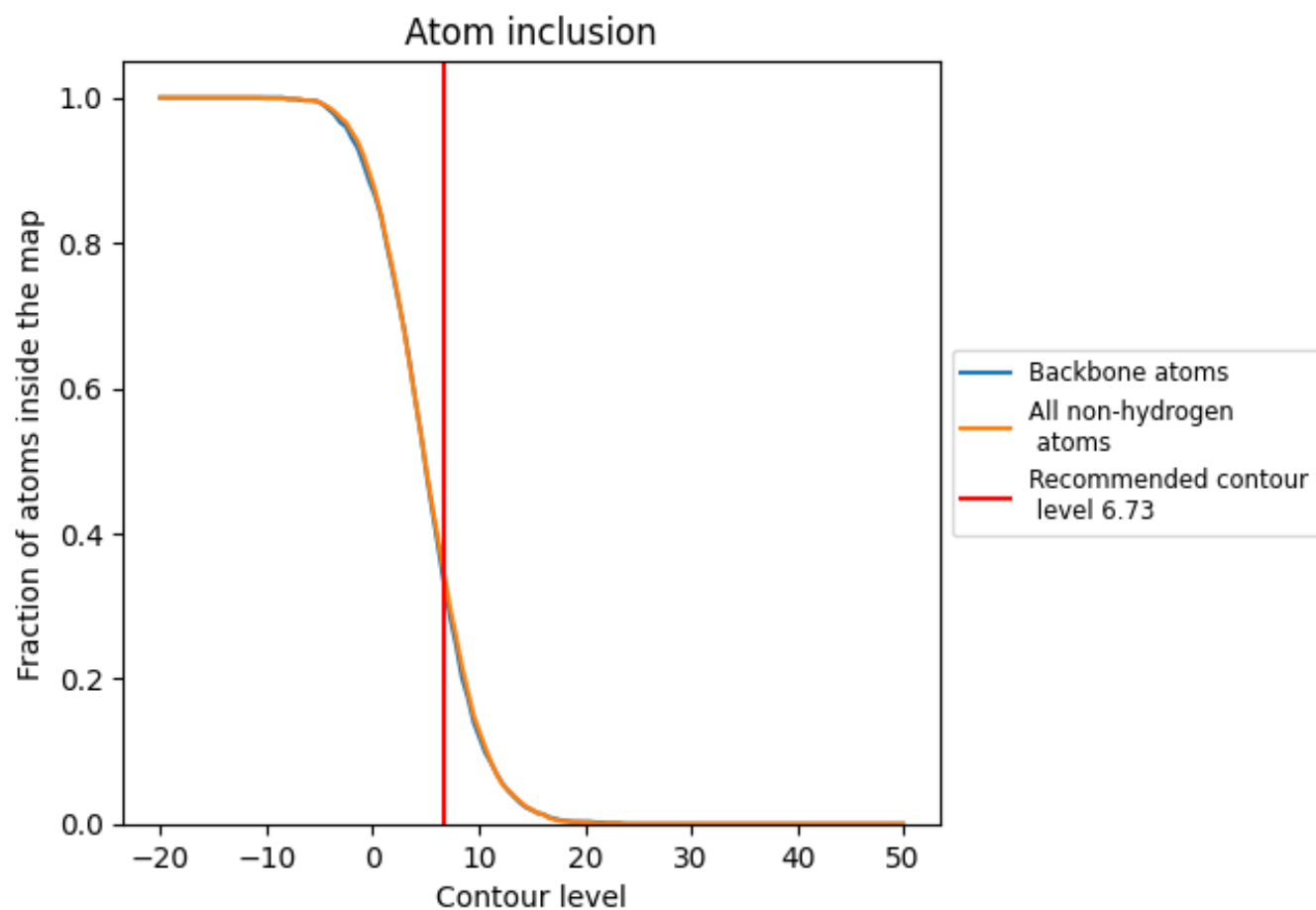
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.73).

9.4 Atom inclusion ⓘ



At the recommended contour level, 33% of all backbone atoms, 34% 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 (6.73) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3430	<div></div> 0.1460
A	<div></div> 0.3450	<div></div> 0.1460

