



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 08:48 PM UTC

PDB ID : 7JGG / pdb_00007jgg
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.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

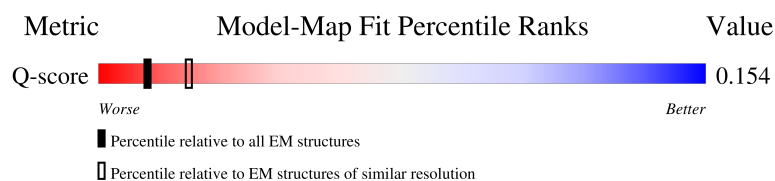
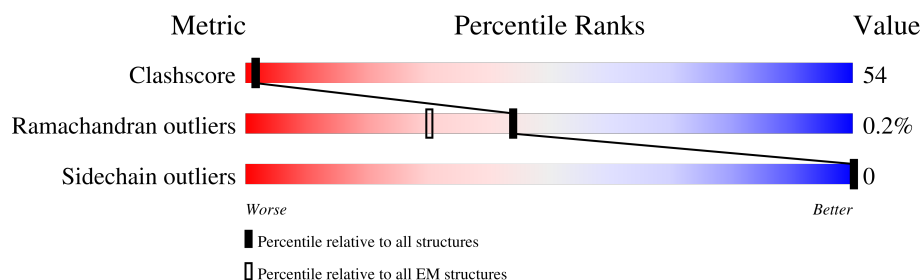
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.88 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1260 (4.38 - 5.38)

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



THR	L2554	K2565	L2497	G2432	L2367	K2305	W2236	P2173	S2104	L2040
GLU	K2566	D2498	D2498	S2433	L2368	E2306	E2237	P2174	D2105	C2041
VAL	K2567	L2499	L2499	I2434	P2369	Q2307	A2238	P2175	M2106	F2042
LYS	E2568	P2500	P2500	I2435	R2370	V2308	I2239	F2176	L2107	S2043
ASN	E2569	N2501	N2501	K2436	R2371	D2309	K2244	L2177	N2108	S2044
CYS	Q2570	D2503	D2503	D2438	R2372	T2310	K2245	R2178	T2109	R2044
MET	S2571	D2504	D2504	MET	K2373	P2311	K2246	W2179	I2110	I2045
CYS	L2572	E2505	E2505	M2441	N2374	E2315	Y2247	I2180	Q2111	P2049
LYS	N2573	D2505	D2505	E2442	L2375	ASP	K2248	K2181	F2112	A2050
PRO	S2574	R2510	R2510	N2443	F2376	VAL	M2249	W2183	D2113	N2050
PRO	Q2575	W2511	W2511	N2444	L2377	ILE	ASP	E2184	D2114	N2051
PRO	D2577	E2514	E2514	S2445	K2378	TYR	ASP	G2185	I2115	L2052
ALA	M2578	W2515	W2515	E2381	D2380	ARG	GLU	N2186	K2116	R2053
SER	N2579	I2449	I2449	E2382	E2381	LEU	PHE	W2187	R2117	W2054
ASN	Y2580	G2450	G2450	S2382	L2383	LYS	LYS	W2188	L2118	L2055
ASN	K2581	K2451	K2451	D2383	T2384	HIS	ASN	C2188	L2119	E2056
GLY	E2582	F2519	F2519	T2384	G2385	GLU	PHE	I2189	D2120	E2057
THR	T2583	C2520	C2520	K2386	K2386	TYR	ASN	Q2190	R2121	F2058
LYS	K2584	T2521	T2521	Y2387	K2388	ASP	ILE	E2192	L2122	K2059
HIS	A2585	D2455	D2455	K2388	R2389	LYS	GLU	E2193	L2123	E2060
HIS	E2586	G2456	G2456	R2389	L2390	GLY	GLU	H2194	E2124	E2061
HIS	K2587	V2457	V2457	L2391	L2391	PRO	PRO	K2195	E2125	E2062
HIS	E2588	G2458	G2458	L2393	L2393	D2331	ASP	E2196	T2127	L2063
E2589	E2588	Q2459	Q2459	F2394	F2394	E2332	ALA	Y2197	K2064	K2064
S2590	E2589	N2460	N2460	K2395	K2395	I2333	GLU	W2198	N2128	G2065
P2591	N2529	E2461	E2461	E2402	E2402	C2334	GLU	K2199	N2129	A2066
E2592	W2531	R2463	R2463	S2404	S2404	T2340	TYR	S2200	T2130	Q2067
Y2593	T2532	K2464	K2464	E2405	E2405	N2335	PRO	E2131	E2131	S2068
F2594	N2535	K2465	K2465	V2406	V2406	K2336	ASN	K2132	K2132	E2069
K2595	S2536	W2466	W2466	S2404	S2404	Y2337	ALA	V2133	V2133	G2070
D2596	A2537	D2467	D2467	E2405	E2405	Y2342	ASN	D2134	D2134	K2071
K2597	K2538	M2468	M2468	V2406	V2406	ASN	LYS	W2135	W2135	F2072
C2598	CYS	N2470	N2470	E2407	E2407	LYS	LYS	D2136	D2136	L2073
N2599	THR	K2471	K2471	R2408	R2408	MET	HIS	N2140	N2140	W2076
E2601	SER	Y2472	Y2472	L2409	L2409	LYS	CYS	K2141	K2141	W2077
C2602	ASN	H2473	H2473	K2410	K2410	LYS	SER	K2142	K2142	E2079
L2605	ASN	I2474	I2474	K2411	K2411	ASN	LYS	S2143	S2143	D2082
S2606	G2544	W2475	W2475	V2412	V2412	ASP	PRO	I2144	I2144	K2083
E2607	S2545	E2476	E2476	Y2413	Y2413	ASP	CYS	W2145	W2145	E2084
TYR	V2546	S2477	S2477	G2414	G2414	THR	CYS	K2153	K2153	K2085
PHE	D2547	M2478	M2478	E2415	E2415	TRP	GLY	K2154	K2154	A2086
LYS	K2548	L2479	L2479	A2416	A2416	THR	ASN	L2087	L2087	L2087
ASP	K2549	K2483	K2483	K2417	K2417	D2354	ASP	E2088	E2088	A2089
GLU	E2550	Y2486	Y2486	T2418	T2418	L2355	MET	M2090	M2090	M2090
THR	C2551	G2487	G2487	K2419	K2419	W2356	GLN	K2091	K2091	K2091
ARG	T2552	ASN	ASN	V2420	V2420	K2357	ILE	I2159	I2159	W2092
TRP	E2553	ILE	ILE	W2421	W2421	N2358	LYS	D2160	D2160	S2093
LYS	K2556	SER	SER	K2424	K2424	S2359	THR	D2161	D2161	S2093
ASN	W2557	GLU	GLU	K2425	K2425	S2360	LYS	P2162	P2162	F2094
PRO	Y2558	ASN	ASN	F2427	F2427	D2361	LYS	S2163	S2163	W2095
GLU	S2559	ASP	ASP	S2428	S2428	ILE	TYR	W2164	W2164	D2096
THR	N2560	ARG	ARG	A2429	A2429	ASN	LYS	E2227	E2227	W2097
LEU	F2561	LYS	LYS	D2430	D2430	LYS	TYR	C2165	C2165	E2098
ASP	L2562	MET	MET	I2431	I2431	V2365	ASP	T2167	T2167	Y2099
								K2231	K2231	I2100
								R2232	R2232	I2101
								G2103	G2103	G2103

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 (Å)	317.4, 317.4, 317.4	wwPDB
Map dimensions	300, 300, 300	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	0.10	0/4264	0.30	0/5710

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.

There are no bond angle outliers.

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	450	0
All	All	4182	28	4095	450	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 54.

The worst 5 of 450 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:2159:ILE:HG13	1:A:2167:ILE:HG22	1.47	0.97

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%)	43 77

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%)	461 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2422	HIS
1	A	2459	GLN
1	A	2506	HIS
1	A	2470	ASN
1	A	2374	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.

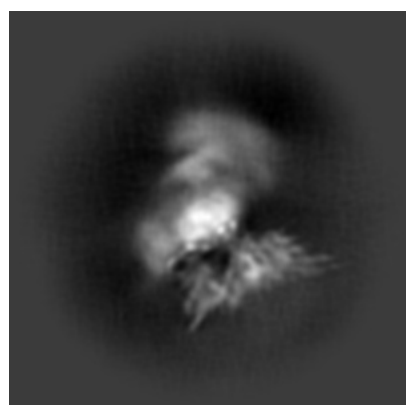
6 Map visualisation [i](#)

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

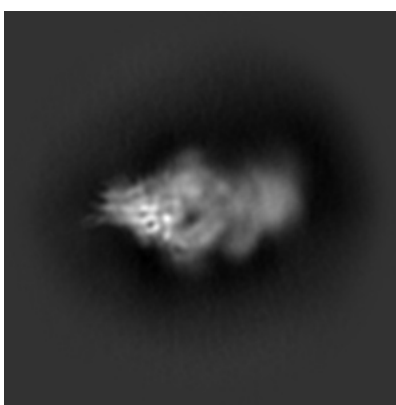
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

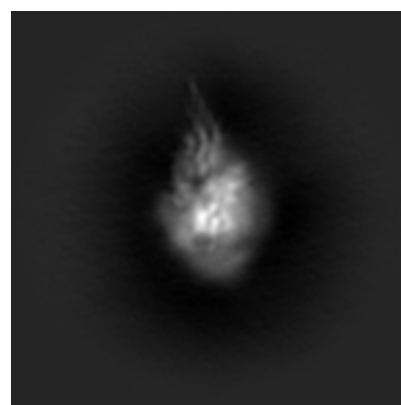
6.1.1 Primary map



X



Y

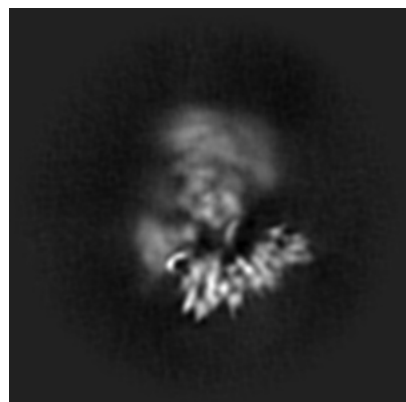


Z

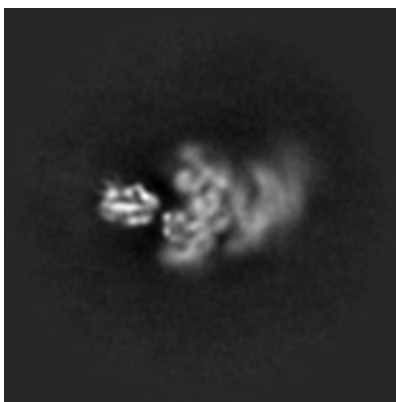
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

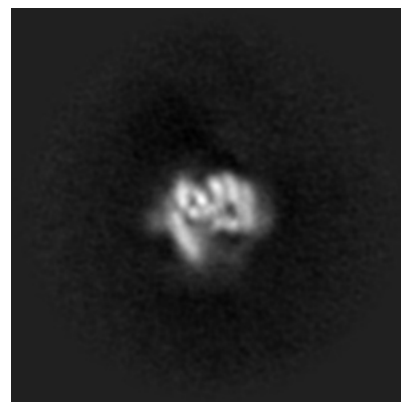
6.2.1 Primary map



X Index: 150



Y Index: 150

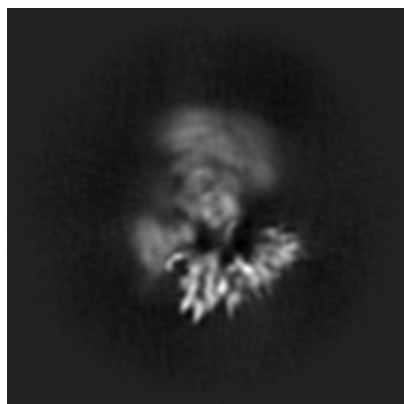


Z Index: 150

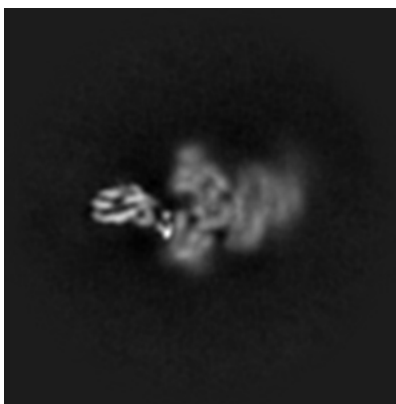
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

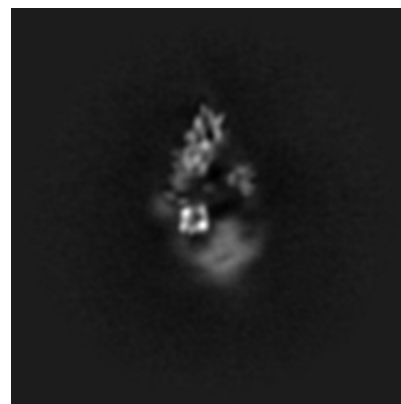
6.3.1 Primary map



X Index: 152



Y Index: 144

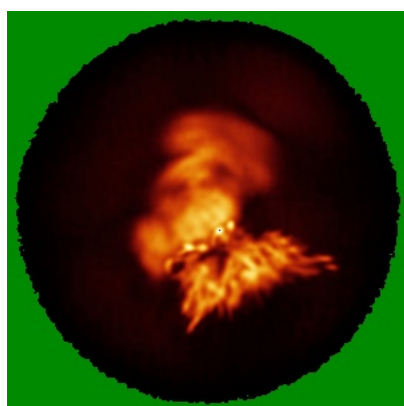


Z Index: 122

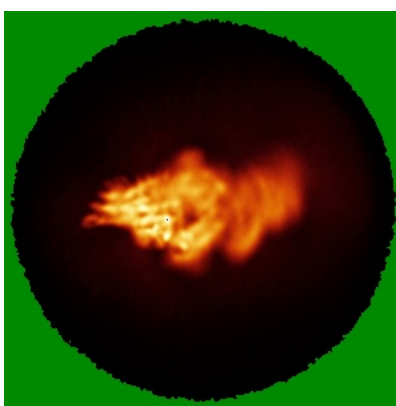
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

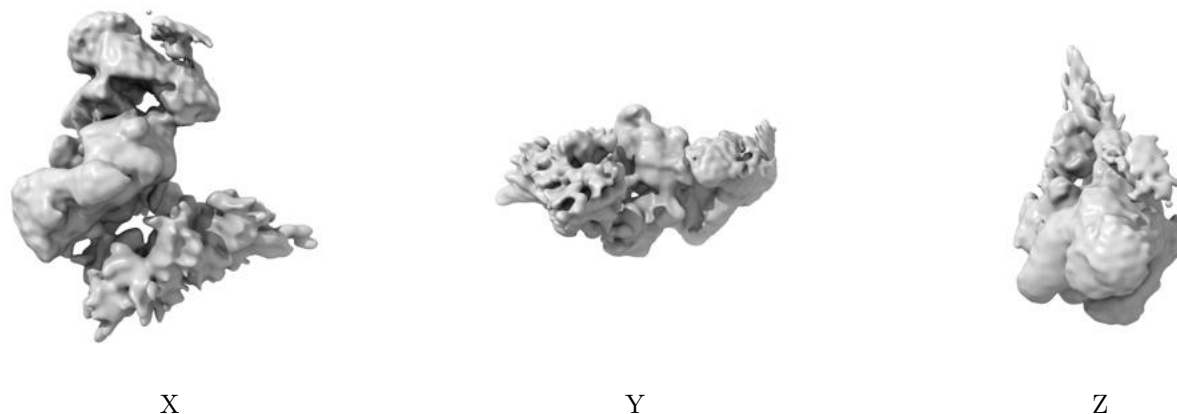


Z

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



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.

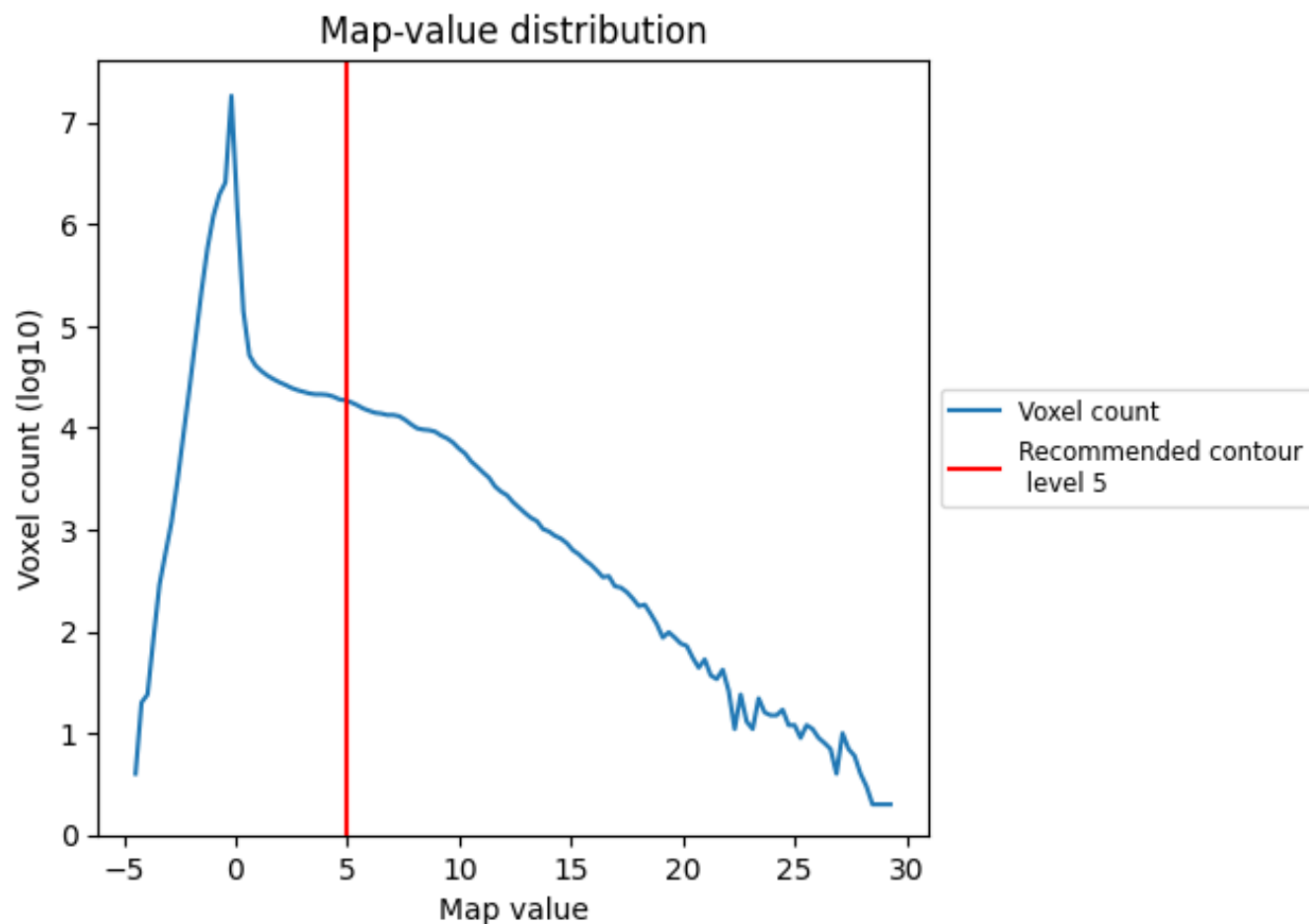
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

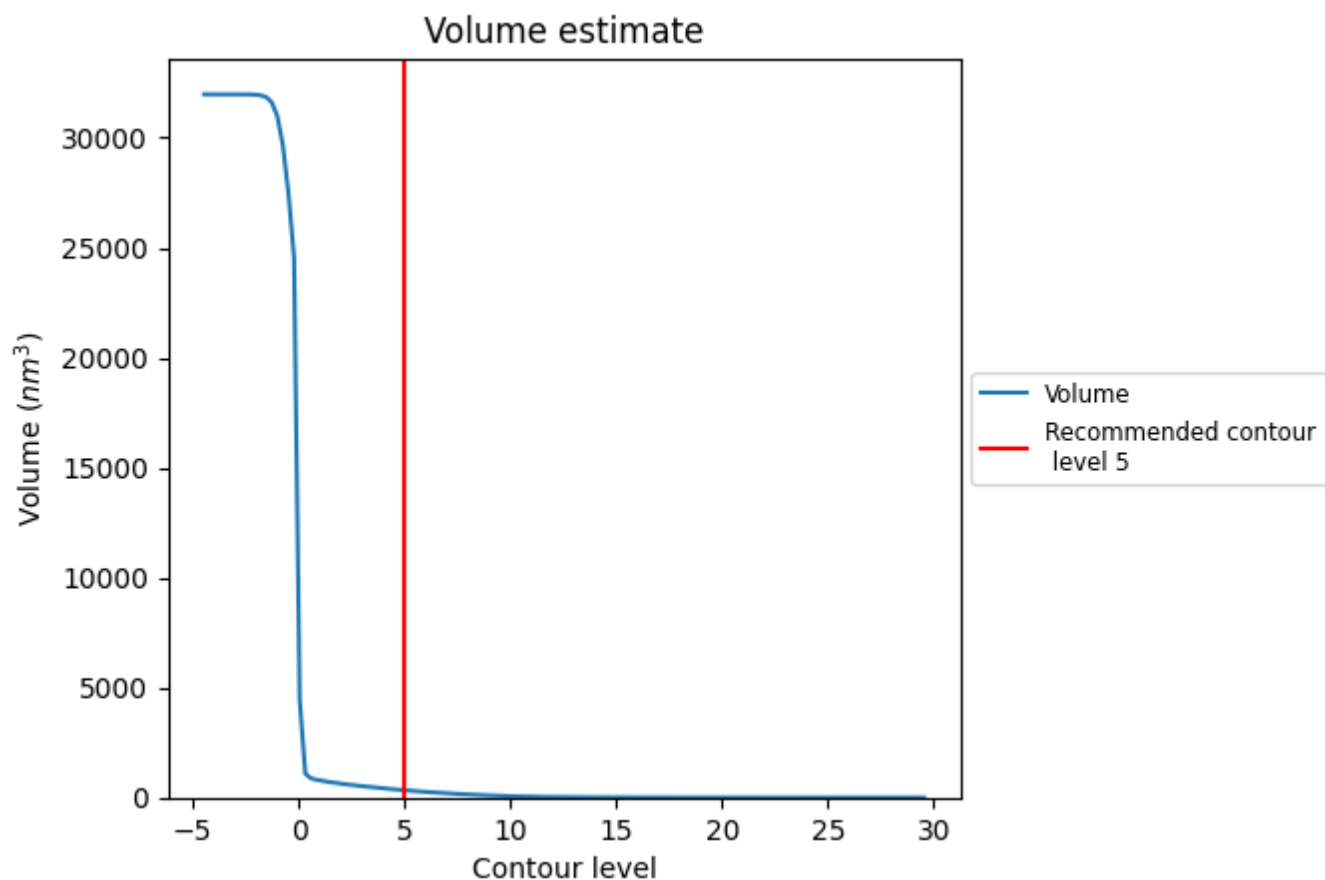
This section contains the results of statistical analysis of the map.

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.

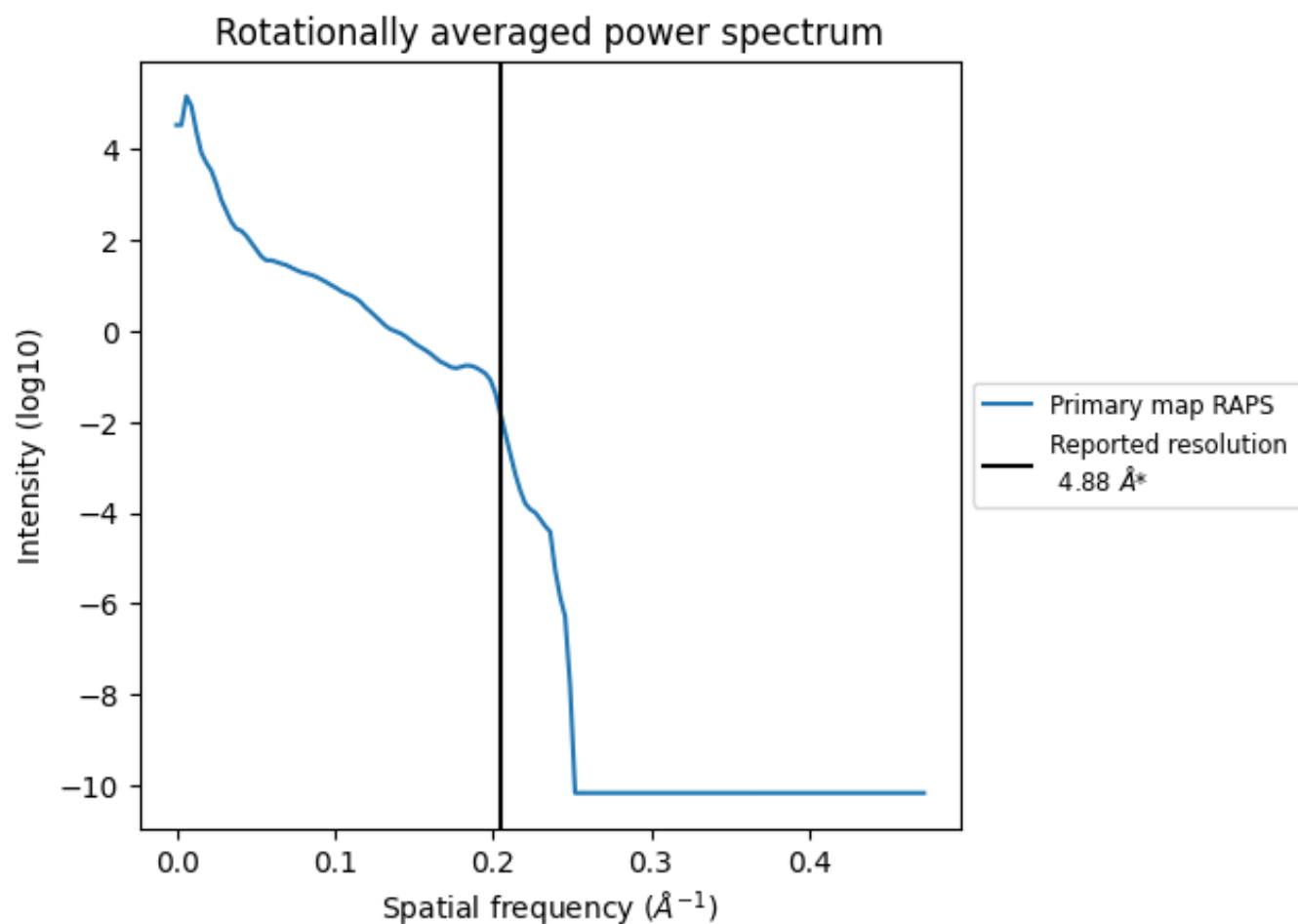
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 332 nm³; 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

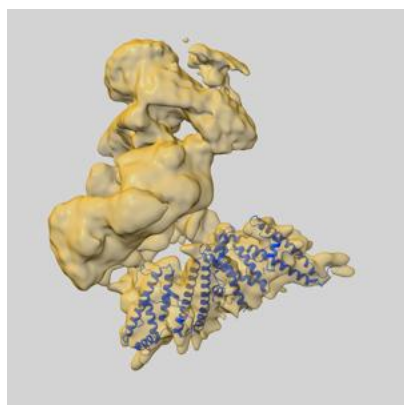
8 Fourier-Shell correlation ⓘ

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

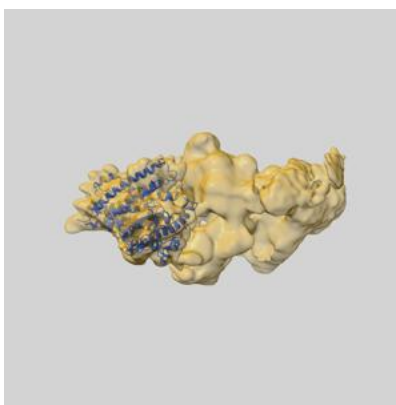
9 Map-model fit [i](#)

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](#).

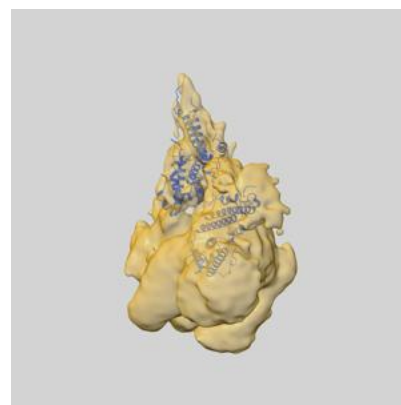
9.1 Map-model overlay [i](#)



X



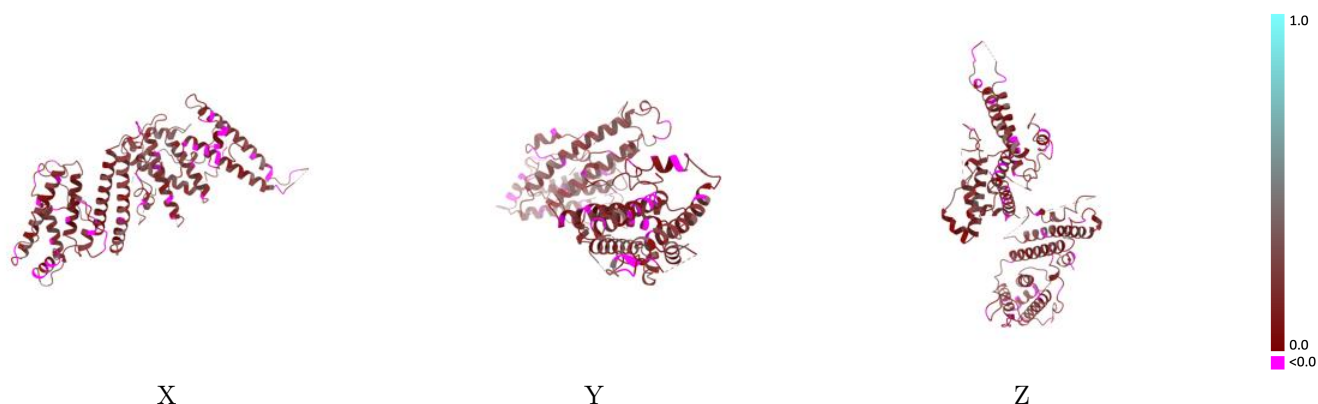
Y



Z

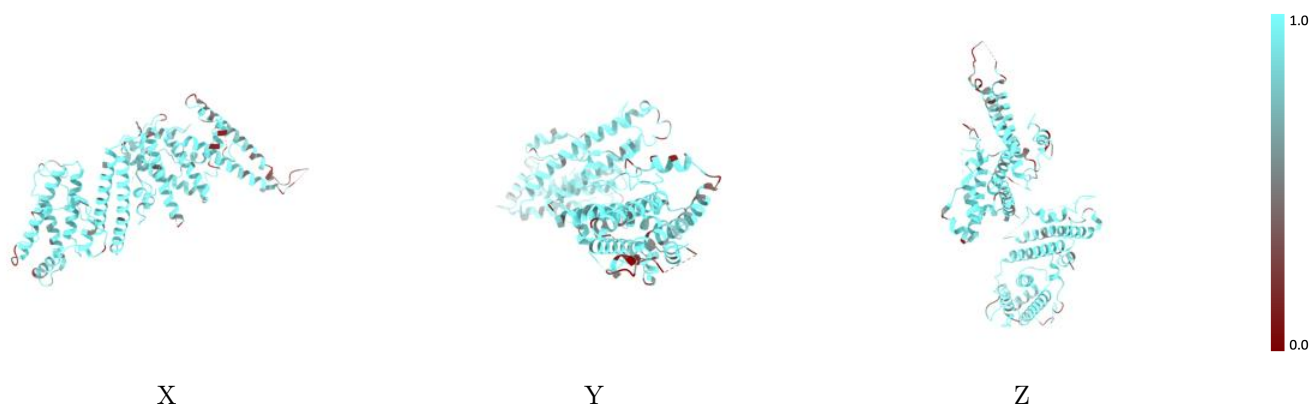
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



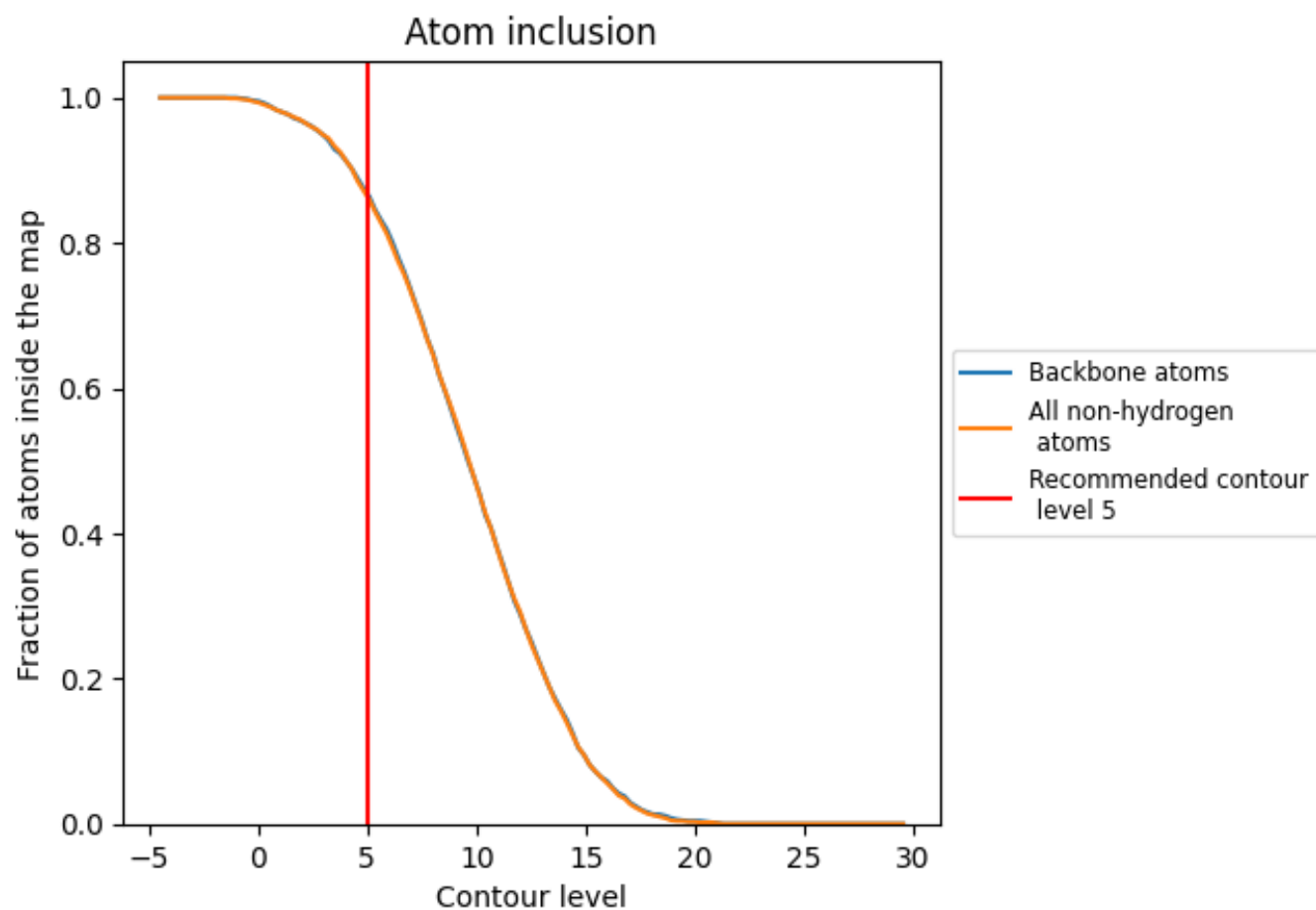
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.8640	0.1540
A	0.8660	0.1540

