



## wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 10:53 am GMT

PDB ID : 7NNH  
EMDB ID : EMD-12477  
Title : Cryo-EM structure of VAR2CSA FCR3 domain DBL5/6  
Authors : Wang, K.T.; Dagil, R.; Salanti, A.; Gourdon, P.E.  
Deposited on : 2021-02-24  
Resolution : 4.00 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

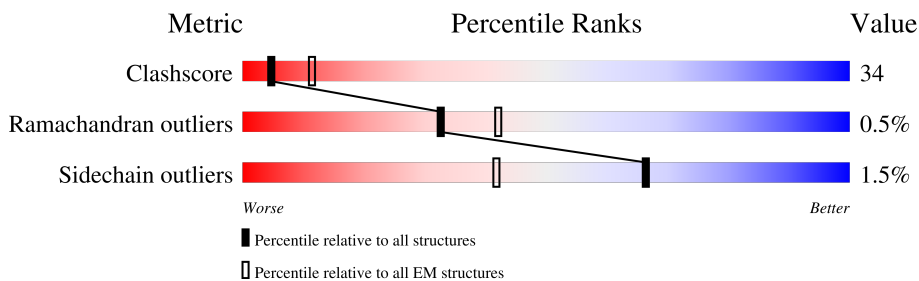
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.00 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	X	2649	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5299 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 Erythrocyte membrane protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	X	637	5299	3332	916	1013	38	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1194	SER	ASN	conflict	UNP Q6UDW7
X	1730	ASN	ASP	conflict	UNP Q6UDW7
X	1878	ASP	GLY	conflict	UNP Q6UDW7
X	2243	GLN	ARG	conflict	UNP Q6UDW7





R2045	R2046	Q2047	L2048	C2049	F2050	S2051	R2052	I2053	W2054	R2055	G2056	F2057	A2058	N2059	L2060	R2061	S2062	N2063	N2064	E2065	F2066	K2067	E2068	E2069	L2070	L2071	K2072	G2073	A2074	Q2075	S2076	E2077	G2078	R2079	F2080	L2081	G2082	N2083	Y2084	Y2085	K2086	E2087	H2088	R2089	D2090	K2091	E2092	Y2103	D2104	D2107	I2108	I2109	K2110	T2112	D2113	R2114	M2117	I2118	E2119	F2120	K2121	D2122	I2123	K2124	I2125	K2126	L2127	D2128	R2129	L2130	K2133	E2134	T2135	N2136	N2137	T2138	K2139	K2140	D2143	W2144	K2146	T2147	N2148	K2149	K2150	S2151	I2152	N2153	N2154	A2155	M2156	L2157	G2158	C2159	I2230	Y2160	K2161	K2162	S2163	G2164	N2165	K2166	D2169	P2170	S2171	I2175	P2176	W2244	E2245	P2182	Q2183	F2184	L2185	R2186	W2187	I2188	K2189	E2190	W2191	W2192	G2193	N2194	C2196	I2197	K2198	K2199	Q2200	E2201	K2202	E2204	V2205	V2206	K2207	S2208	K2209	C2210	S2211	T2214	G2217	A2218	Q2219	A2220	N2224	N2225	C2226	T2227	S2228	E2229	I2230	K2231	K2232	Y2233	Q2234	E2235	W2236	S2237	K2238	K2239	R2240	S2241	T2242	W2244	E2245	T2246	I2247	W2248	E2249	F2300	K2301	Q2302	I2303	K2304	E2305	Q2306	V2307	K2308	I2309	P2310	L2313	E2314	D2315	V2316	I2317	Y2318	R2319	I2320	K2321	H2322	H2323	E2324	Y2325	D2326	K2327	G2328	Y2331	I2332	K2333	N2334	K2335	Y2336	K2337	K2338	N2339	H2340	D2341	R2342	M2343	K2344	F2350	V2351	T2352	D2353	N2354	F2355	V2356	K2357	K2358	E2361	I2362	S2363	N2364	E2365	V2366	L2367	I2368	P2369	P2370	R2371	R2372	L2374	N2375	F2381	S2382	K2383	L2384	C2385	W2386	E2387	K2388	K2389	L2393	F2394	K2395	Y2399	W2400	F2403	T2404	E2405	R2408	L2409	G2414	R2417	W2421	H2422	A2423	H2424	K2425	Y2426	S2427	F2428	T2431	G2432	S2433	D2438	D2439	M2440	M2441	E2442	K2443	N2444	S2445	S2446	D2447	K2448	L2449	G2450	K2451	I2452	L2463	T2464	D2465	M2469	N2470	K2471	Y2472	M2476	L2479	Y2482	R2483	E2484	A2485	E2486	G2487	D2488	T2489	E2490	T2491	N2492	E2493	M2494	C2495	R2496	F2497	V2503	P2504	Q2505	F2506	L2507	R2508	W2509	F2510	W2513	F2517	C2518	D2519	R2520	R2521	Q2522	K2523	L2524	Y2525	D2526	D2528	K2529	L2528	N2529	S2530	E2531	C2532	I2533	S2534	A2535	E2536	C2537	T2538	N2539	G2540	S2541	V2542	D2543	N2544	S2545	K2546	C2547	T2548	H2549	A2550	C2551	N2552	N2553	Y2554	K2555	N2556	Y2557	I2558	K2561	K2562	E2563	F2564	Y2565	E2566	T2567	Q2568	T2569	N2570	D2573	N2574	E2575	F2576	K2577	N2578	K2579	N2580	P2581	S2582	D2583	K2584	D2585	A2586	F2587	D2588	Y2589	L2590	K2591	E2592	K2593	C2594
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	97695	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.403	Depositor
Minimum map value	-0.505	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.53	Depositor
Map size (Å)	365.19998, 365.19998, 365.19998	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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	X	0.28	0/5414	0.59	2/7269 (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	X	0	10

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	X	2279	CYS	C-N-CD	-6.08	107.22	120.60
1	X	2326	ASP	N-CA-C	5.17	124.96	111.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	2253	LYS	Peptide
1	X	2284	ASN	Peptide
1	X	2290	ASN	Peptide
1	X	2297	LYS	Peptide
1	X	2302	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	X	5299	0	5167	354	0
All	All	5299	0	5167	354	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 34.

The worst 5 of 354 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:X:2368:ILE:HG21	1:X:2441:MET:HB3	1.56	0.87
1:X:2199:LYS:NZ	1:X:2281:CYS:SG	2.47	0.87
1:X:2338:ASN:HA	1:X:2342:ARG:HH21	1.40	0.84
1:X:2234:GLN:HE21	1:X:2238:ARG:HG3	1.47	0.79
1:X:2290:ASN:OD1	1:X:2292:ASN:ND2	2.16	0.77

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	X	635/2649 (24%)	486 (76%)	146 (23%)	3 (0%)	29 67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	1993	CYS
1	X	1994	PHE
1	X	2077	GLU

### 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	X	589/2404 (24%)	580 (98%)	9 (2%)	65 80

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	2449	ILE
1	X	2529	ASN
1	X	2166	LYS
1	X	2189	LYS
1	X	2319	ARG

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

Mol	Chain	Res	Type
1	X	2083	ASN
1	X	2202	HIS
1	X	2234	GLN
1	X	2291	ASN
1	X	2570	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 monosaccharides 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.

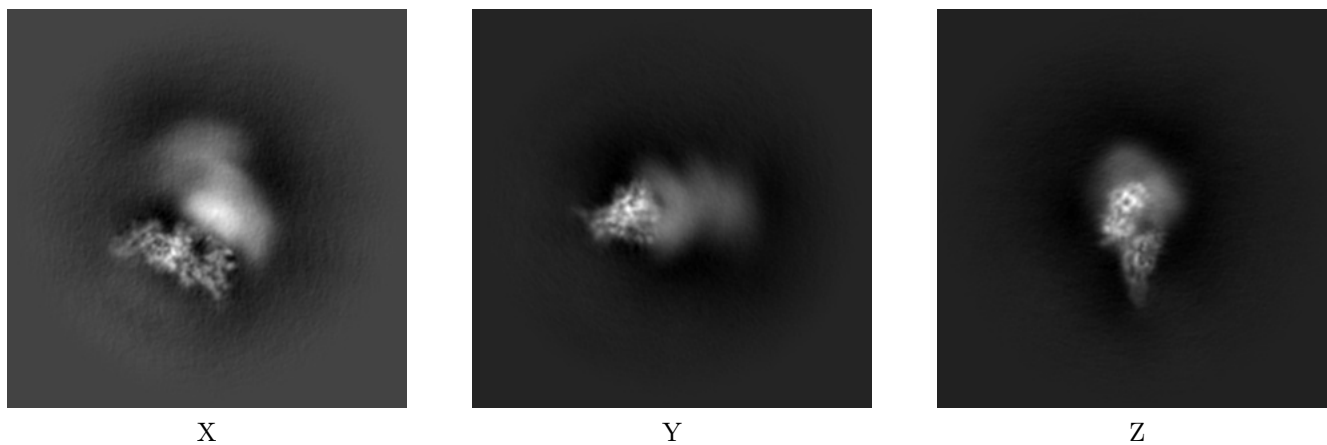
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12477. 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](#)

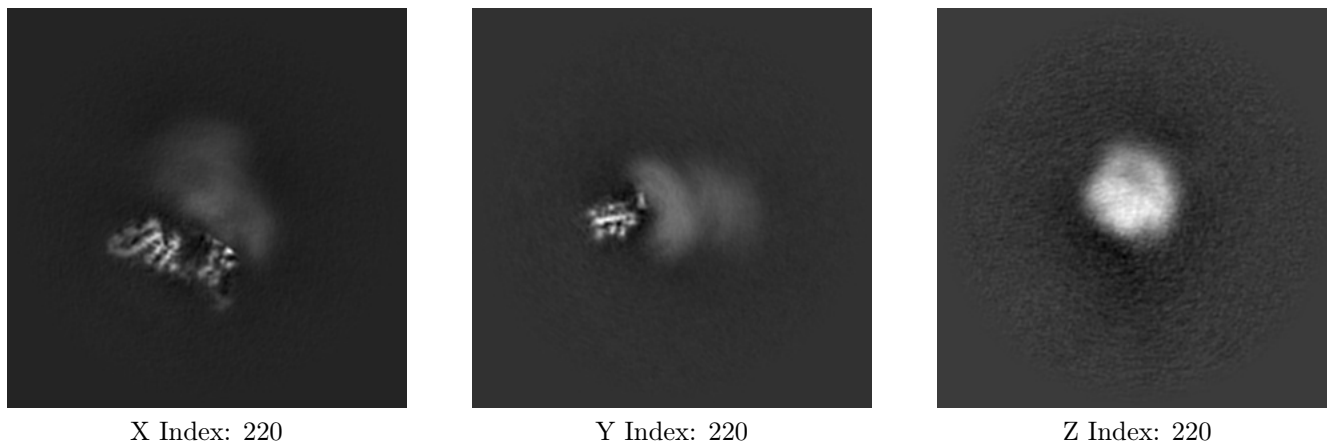
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

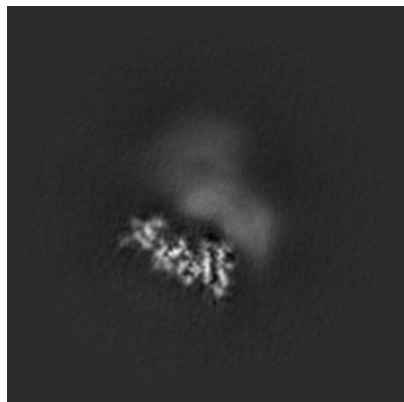
#### 6.2.1 Primary map



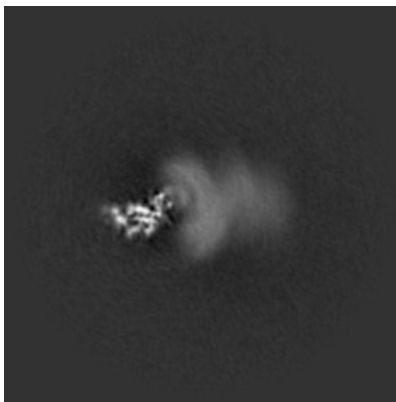
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

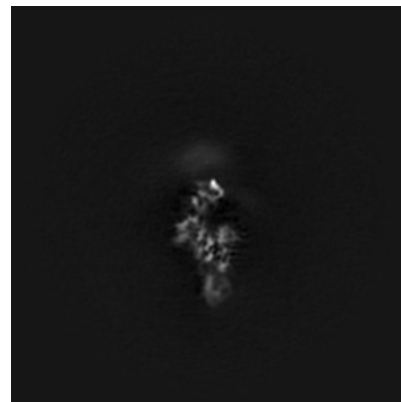
### 6.3.1 Primary map



X Index: 208



Y Index: 231

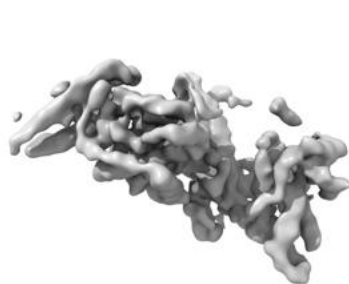


Z Index: 171

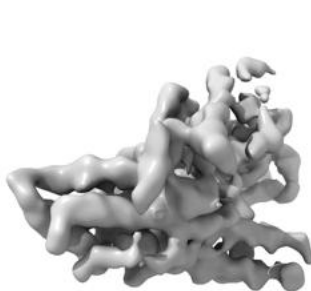
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

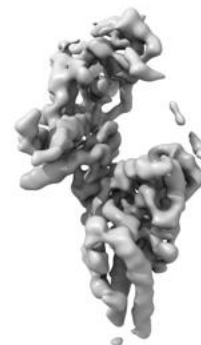
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.53. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

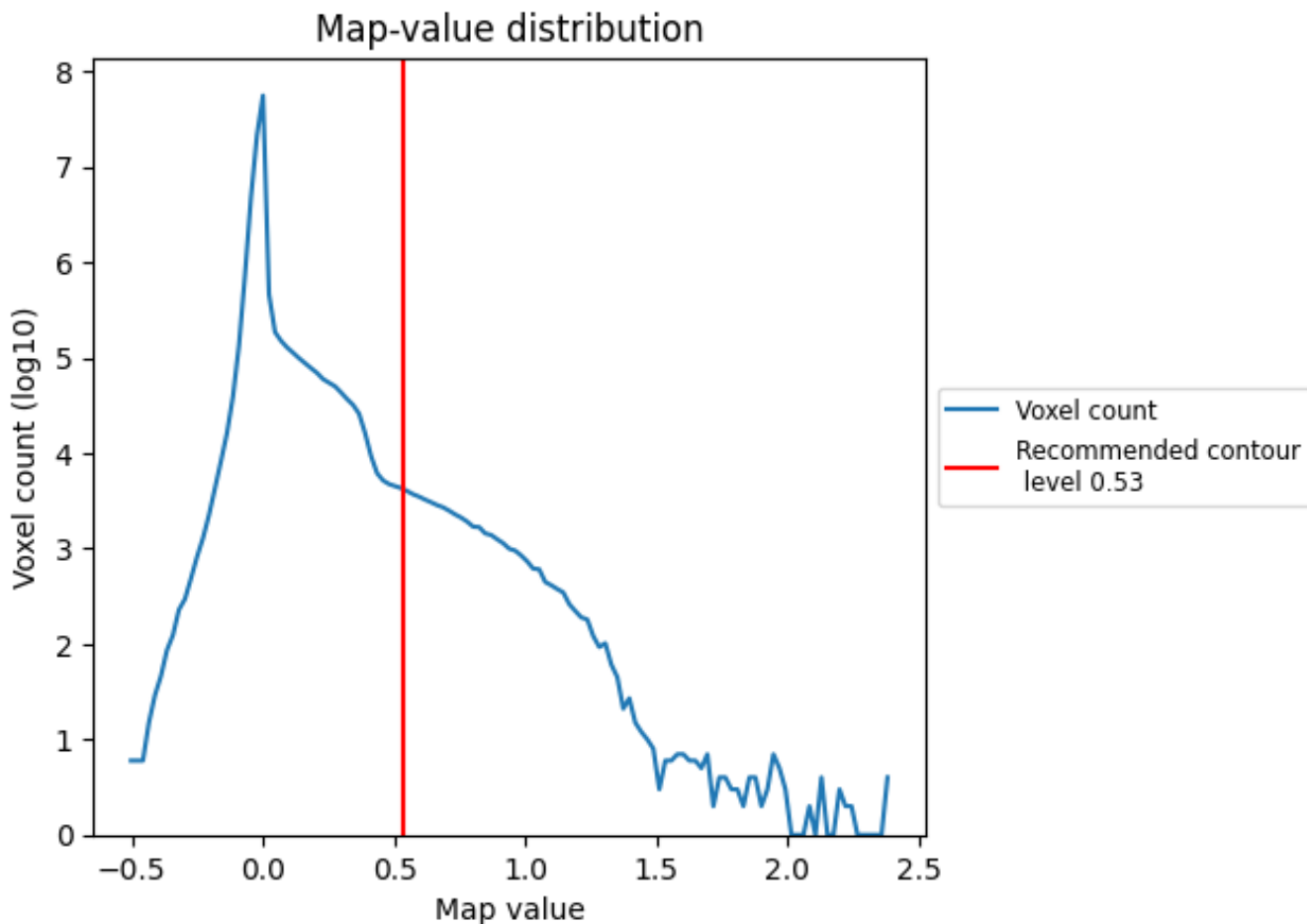
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

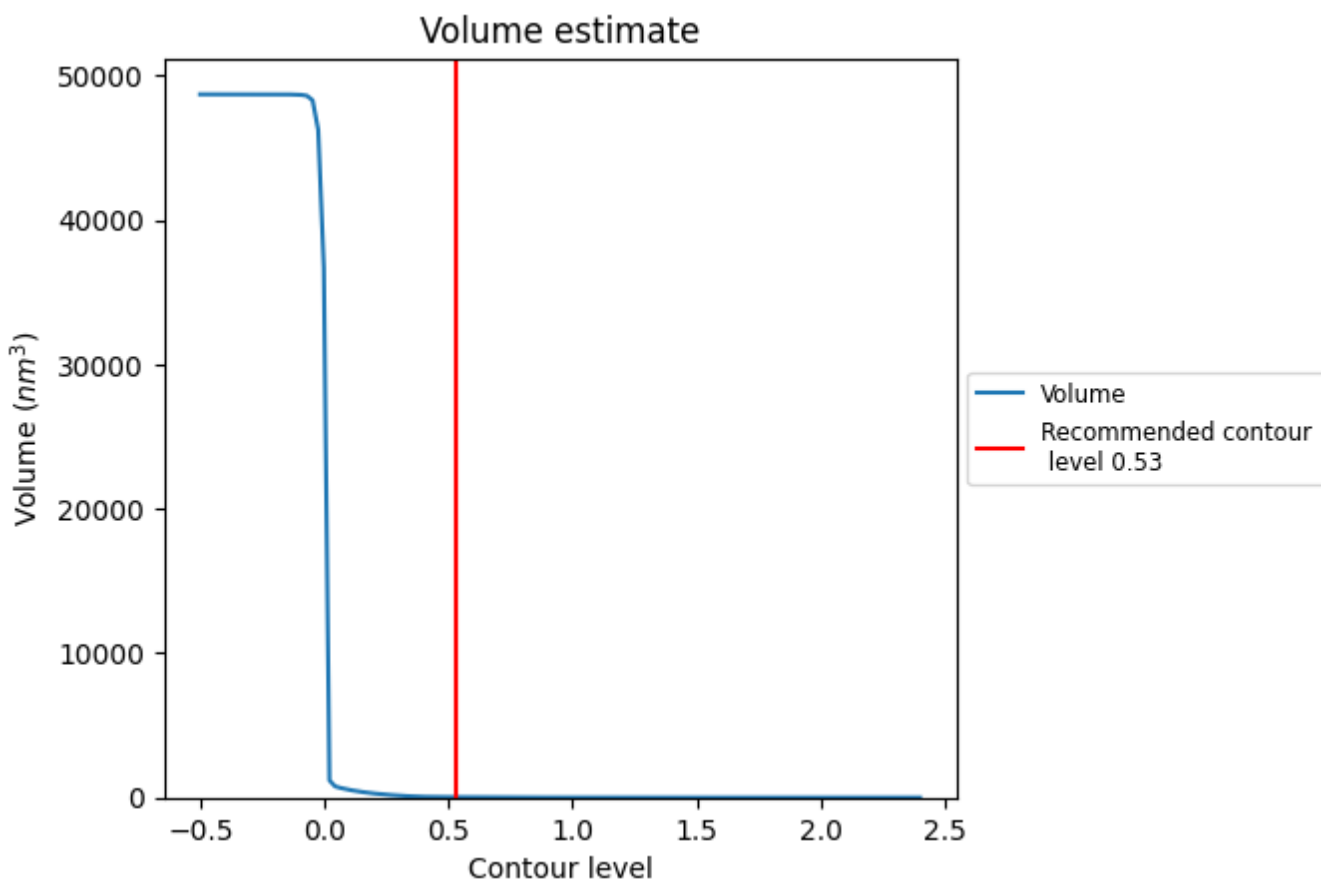
This section contains the results of statistical analysis of the map.

### 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](#)

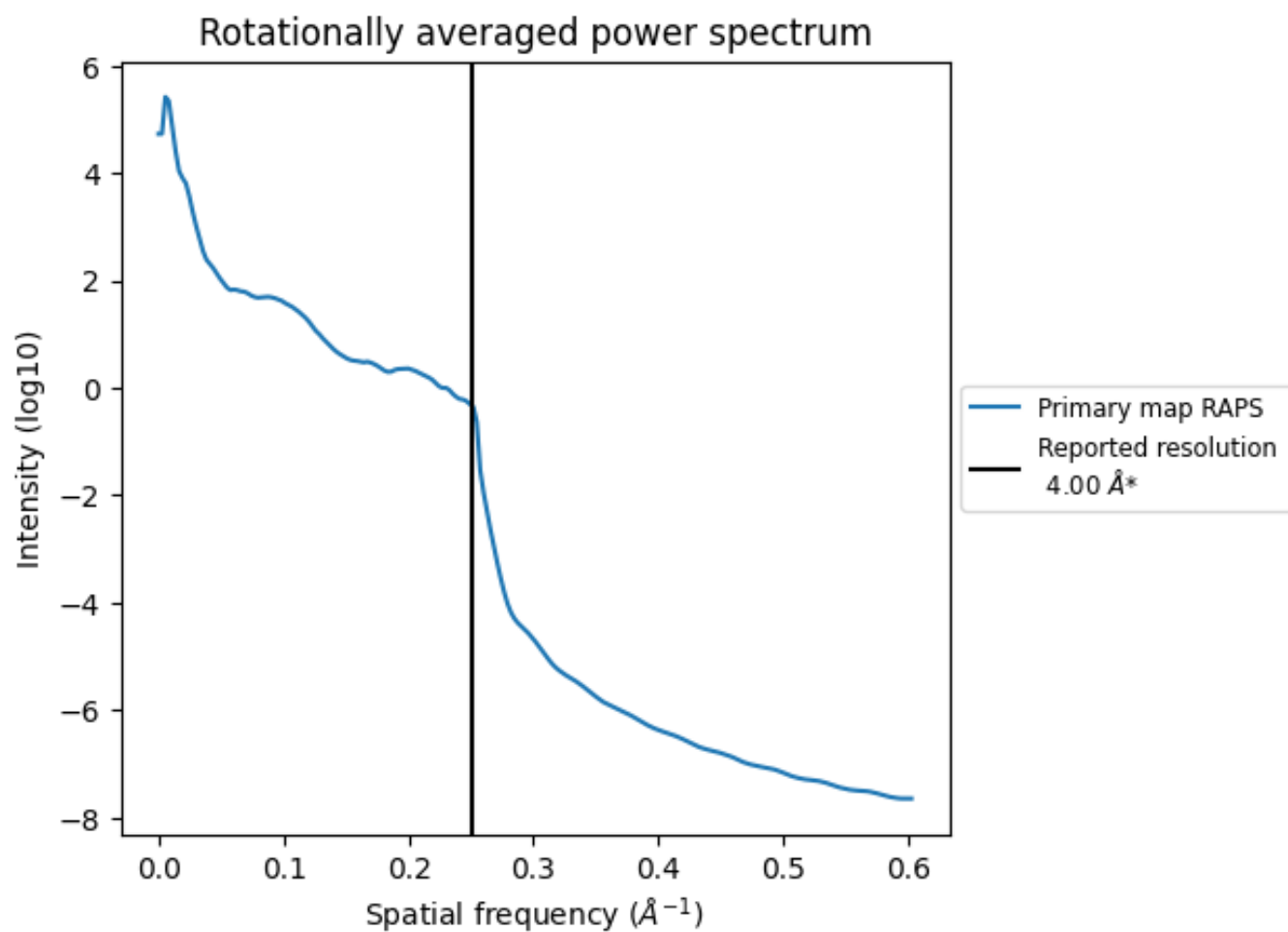


The volume at the recommended contour level is 30 nm<sup>3</sup>; this corresponds to an approximate mass of 27 kDa.

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 [i](#)

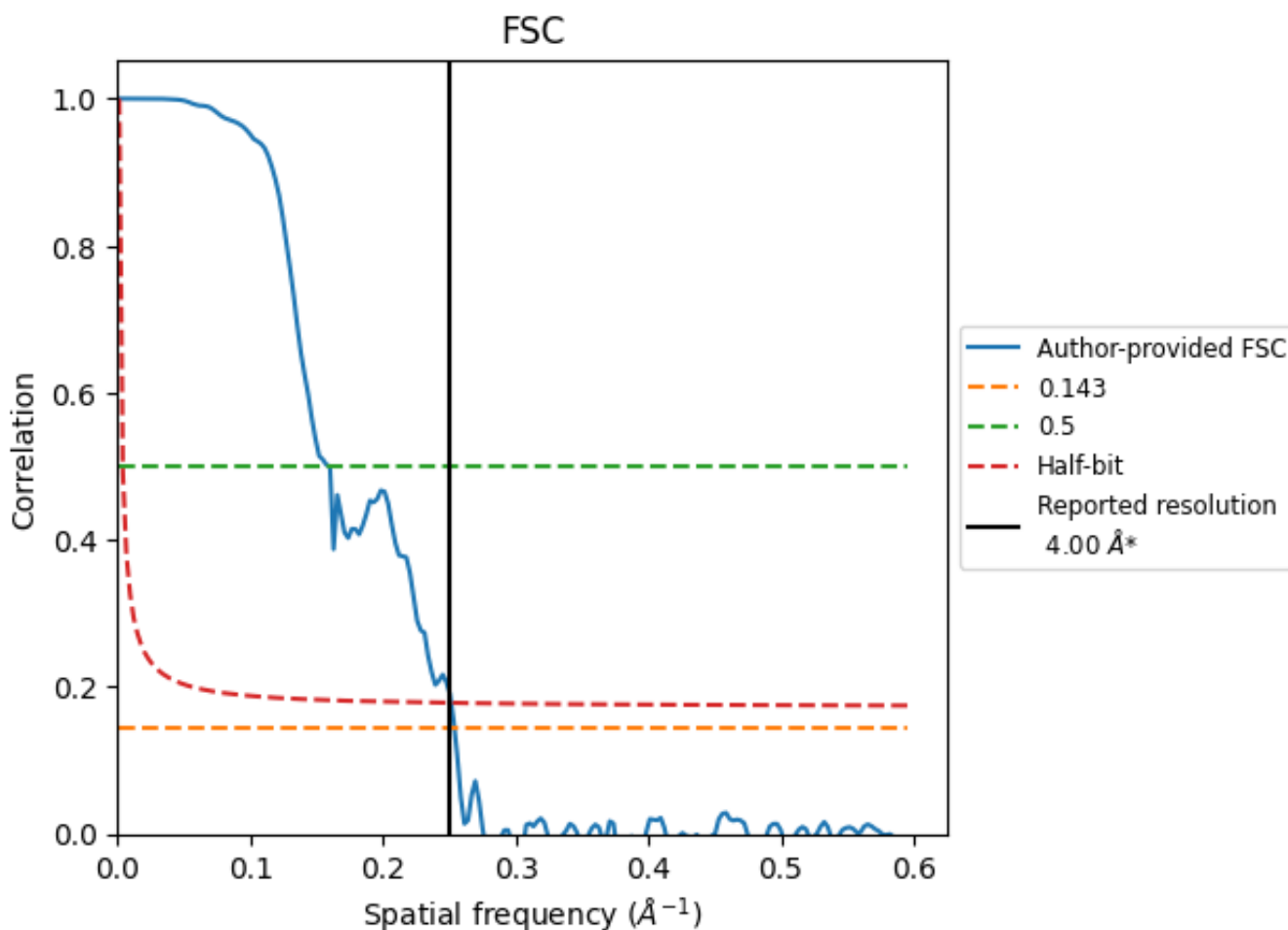


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 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  $0.250 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

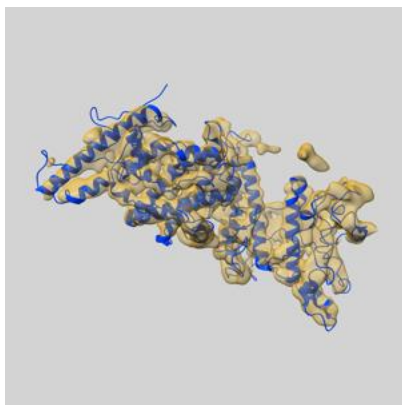
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.94	6.27	3.98
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

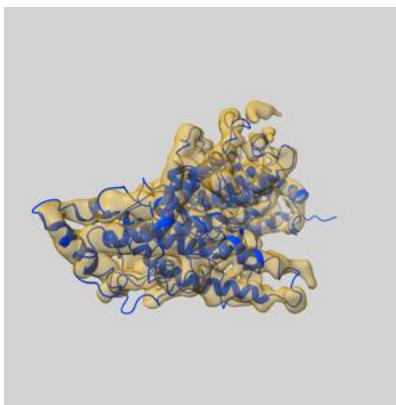
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12477 and PDB model 7NNH. Per-residue inclusion information can be found in section [3](#) on page [4](#).

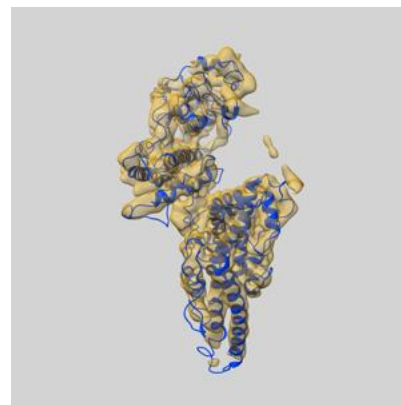
### 9.1 Map-model overlay [i](#)



X



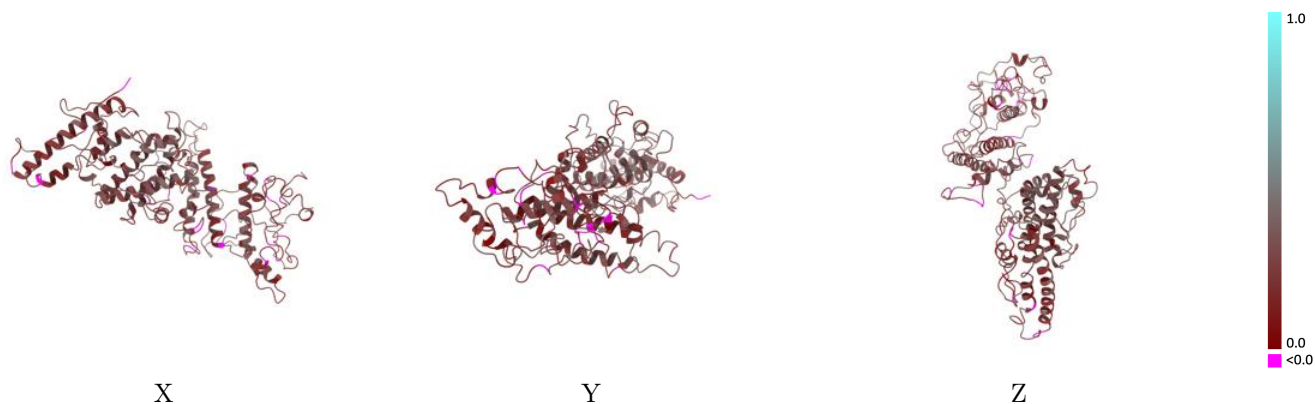
Y



Z

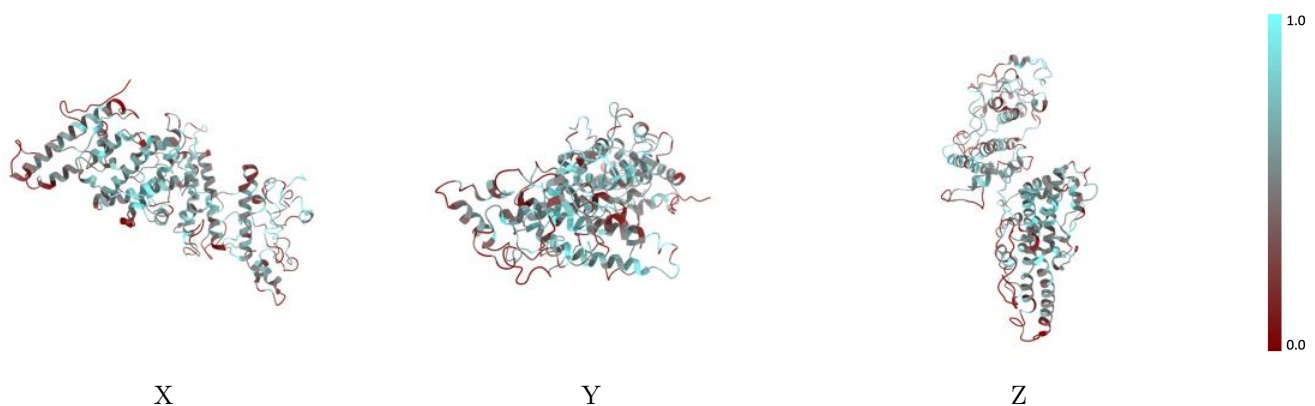
The images above show the 3D surface view of the map at the recommended contour level 0.53 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



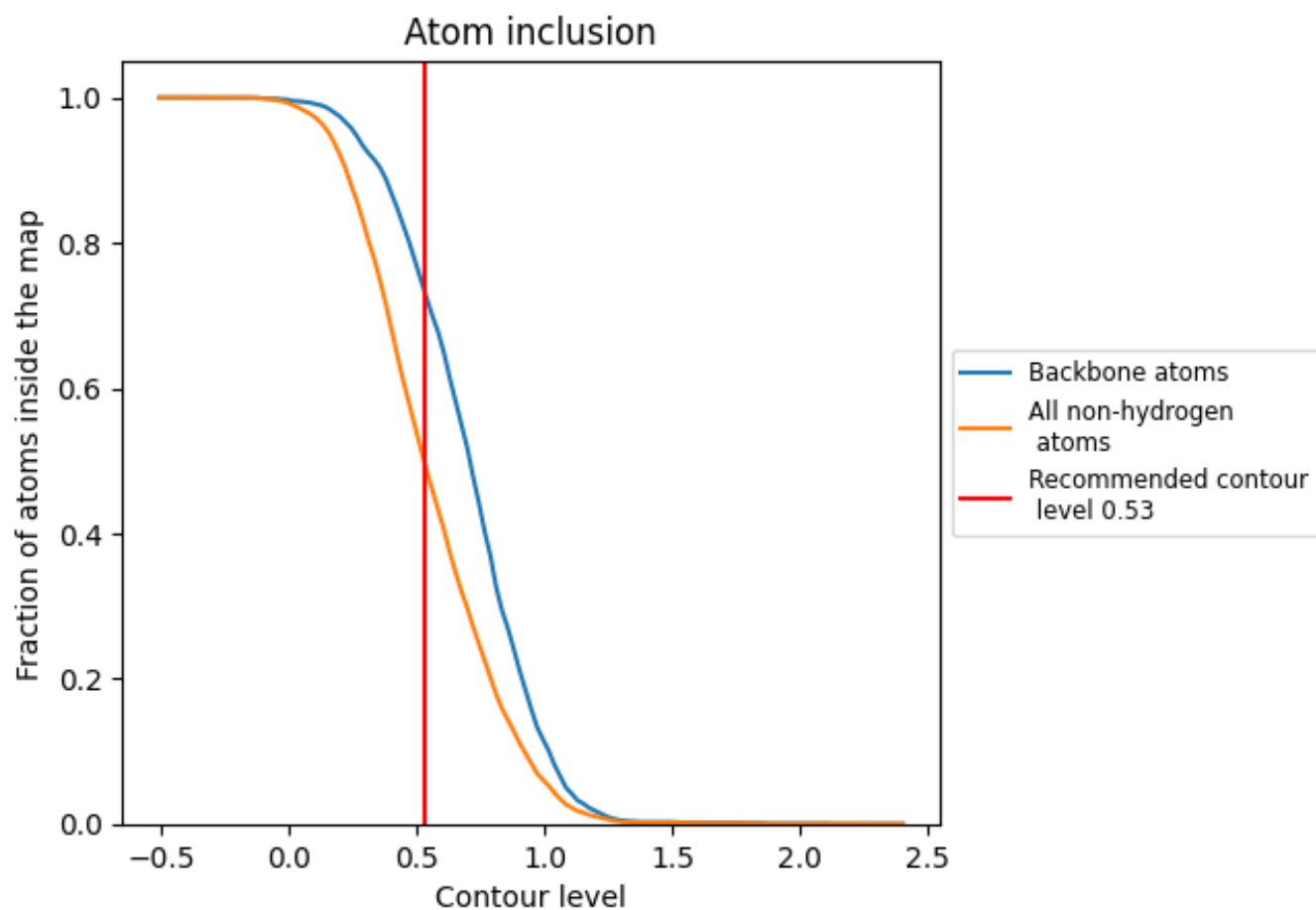
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.53).





## 9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 50% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.53) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4996	 0.2380
X	 0.4996	 0.2380

