



wwPDB EM Validation Summary Report ⓘ

Jul 15, 2025 – 01:17 pm BST

PDB ID : 9QB8 / pdb_00009qb8
EMDB ID : EMD-52990
Title : Lymphostatin - Conformation II - pH 8 Hepes
Authors : Bottcher, B.; Schneider, R.; Griessmann, M.; Ramussen, T.
Deposited on : 2025-02-28
Resolution : 3.40 Å(reported)
Based on initial model : 9euw

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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

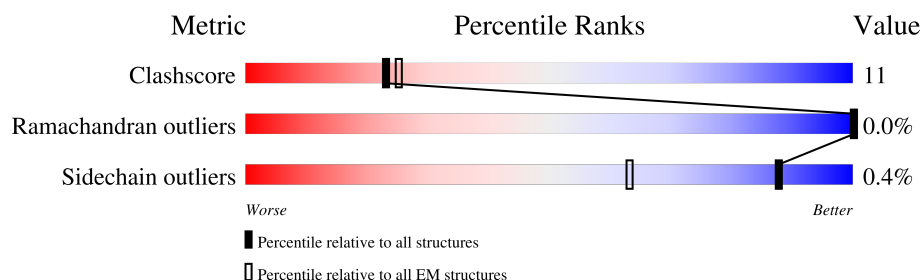
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	3223	 65% 21% 13%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 22339 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.

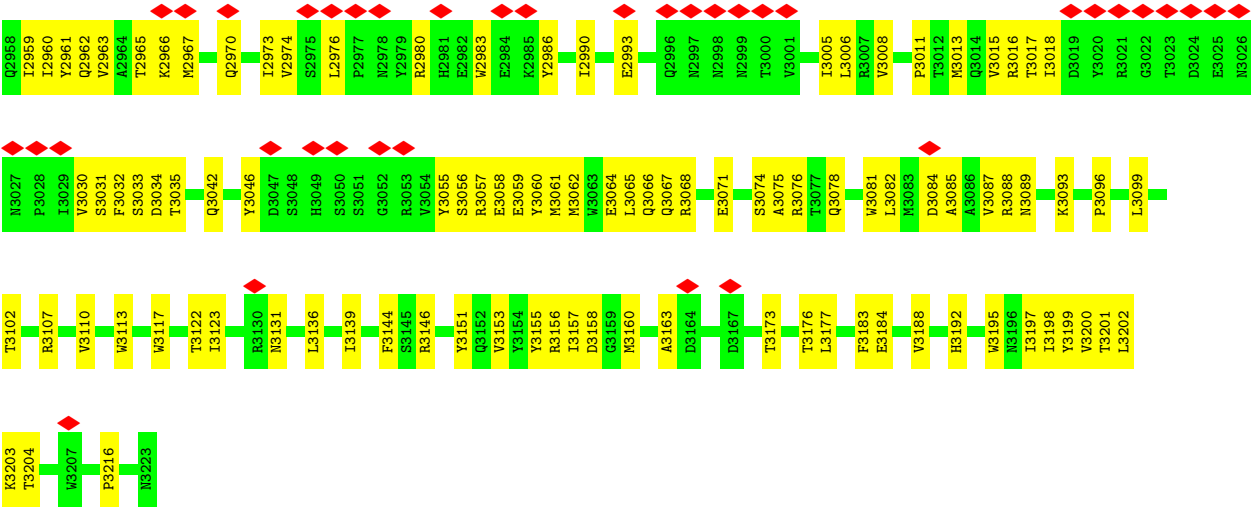
- Molecule 1 is a protein called Lymphostatin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2803	Total	C	N	O	S	0	0
			22338	14119	3874	4269	76		

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Mn	0
			1	1	

GLY	ALA	E2823	V2654	L2555	A2461	N2303	I2115	G1861	L1654	F1403	P1248	SER	GLY	LEU
MET	V2824	E2759	S2657	L2556	I2462	T2304	V2119	I1862	I1685	F1414	E1251	ASN	ILE	GLU
LYS	N2825	A2760	E2658	E2557	L2463	T2305	G2120	M1863	T1686	T1414	T1685	THR	THR	ILE
LYS	D2826	P2761	L2664	S2559	D2464	Q2307	Y2121	F1865	L1699	S1427	P1256	GLU	THR	THR
THR	T2827	L2763	E2665	P2560	R2465	L2310	N2137	L1867	T1709	F1454	V1256	LYS	PHE	PHE
ASP	T2828	L2764	N2666	Y2561	W2469	L2311	W2140	G1868	T1713	R1479	L1257	ASP	ILE	ILE
GLY	D2829	L2765	V2674	L2562	V2477	T2312	P2141	M1869	T1713	R1479	N1262	HIS	GLU	GLU
PRO	R2830	E2766	E2675	E2563	R2478	L2313	R2142	V1870	L1716	M1481	P1264	TYR	ASN	ASN
SER	E2831	E2767	G2676	E2564	F2479	V2314	Y2159	V1872	Q1736	L1485	G1273	ASP	ASP	ASP
VAL	E2832	R2768	K2682	L2573	S2487	A2317	Y2159	G1873	Q1736	L1485	G1273	ARG	PHE	PHE
GLU	L2833	R2770	K2682	L2574	Y2488	K2320	N2166	V1874	Q1736	L1485	G1273	LEU	LEU	LEU
ASP	E2834	S2774	W2687	T2575	Y2488	K2320	N2166	I1885	I1740	L1488	K1274	LEU	ARG	ARG
ASP	K2835	S2775	K2688	L2576	Y2488	D2329	I2169	G1885	R1741	Q1489	V1279	GLY	GLU	GLU
ASP	D2836	A2689	A2577	T2578	Q2494	D2329	I2169	I1885	K1742	Q1489	V1280	ILE	ILE	ILE
ASP	L2837	K2777	E2690	Y2581	L2495	S2343	R2191	ASP	T1746	S1497	V1281	GLU	GLU	GLU
ASP	R2838	T2778	E2692	L2585	V2496	L2364	T2202	THR	R1754	E1501	S1282	ALA	ALA	ALA
ASP	P2839	T2779	V2695	L2590	R2502	N2347	N2198	THR	R1754	E1501	T1295	VAL	VAL	VAL
ASP	L2840	L2781	V2695	L2590	Y2503	N2348	S2199	LEU	M1760	K1517	Y1303	ASN	ASN	ASN
ASP	L2841	L2782	I2699	L2594	S2504	T2358	C2201	LYS	M1528	M1528	N1304	MET	MET	MET
ASP	L2842	L2783	L2702	P2595	E2505	L2364	T2202	ILE	T1784	M1537	I1305	ASN	ASN	ASN
ASP	G2843	M2784	L2702	P2595	E2505	L2364	T2202	ASN	Q1772	M1537	H1306	SER	SER	SER
ASP	D2844	L2785	F2714	L2602	A2509	H2371	L2212	ALA	Q1772	Y1545	N1308	HIS	HIS	HIS
ASP	T2845	H2786	V2720	Q2603	R2512	K2384	L2215	M1897	L1775	Y1545	N1308	GLU	GLU	GLU
ASP	H2846	Q2787	L2721	Q2605	H2513	L2392	P2223	D1898	R1802	T1547	L1314	LEU	LEU	LEU
ASP	R2847	Q2788	P2730	D2606	T2516	L2392	P2223	I1899	F1797	R1573	N1315	PHE	PHE	PHE
ASP	P2848	M2789	L2731	L2613	A2517	I2393	T2226	K1917	Q1798	A1574	N1318	GLU	GLU	GLU
ASP	T2849	L2790	K2732	L2614	G2522	Y2394	E2227	R1943	N1799	I1576	L1319	ILE	ILE	ILE
ASP	N2850	L2792	L2733	R2615	P2522	N2399	L2230	R1957	L1808	S1577	L1322	LYS	LYS	LYS
ASP	A2851	D2793	T2734	P2618	S2524	P2404	K2236	V1963	E1811	Y1592	L1323	GLN	GLN	GLN
ASP	L2852	R2795	S2735	D2619	R2525	K2409	L2239	V1963	E1811	Y1592	L1323	ASN	ASN	ASN
ASP	T2853	R2795	A2736	N2620	Y2525	L2410	L2239	L1968	A1816	P1607	L1332	THR	THR	THR
ASP	L2854	L2797	Q2737	Q2625	R2529	N2411	V2250	L1978	A1816	P1607	L1332	GLN	GLN	GLN
ASP	H2855	L2797	E2738	L2626	M2529	H2412	V2250	Y1974	R1822	F1612	T1337	ASP	ASP	ASP
ASP	L2856	R2799	M2739	F2627	K2530	G2424	T2268	L1978	F1823	I1614	L1340	LEU	LEU	LEU
ASP	N2857	R2800	Q2740	T2632	P2531	G2424	T2268	L1978	F1823	I1614	L1340	THR	THR	THR
ASP	N2858	L2801	L2741	T2633	V2532	M2425	L2268	T1984	N1824	I1618	L1340	LYS	LYS	LYS
ASP	L2859	F2802	E2742	T2634	T2533	T2426	L2268	T1984	N1824	I1618	L1340	GLN	GLN	GLN
ASP	A2860	R2805	R2744	R2637	Q2535	I2436	S2270	F1998	R1828	Q1625	H1356	LEU	LEU	LEU
ASP	E2861	E2806	Q2745	L2638	I2536	L2442	E2276	V2036	T1832	E1626	T1369	LEU	LEU	LEU
ASP	T2862	Q2807	Q2746	E2639	T2539	L2442	E2276	V2036	T1832	E1626	T1369	GLN	GLN	GLN
ASP	L2863	L2808	Q2747	N2640	Q2540	R2447	L2281	Q2045	H1834	E1645	G1376	LEU	LEU	LEU
ASP	R2864	G2809	Q2748	M2642	L2543	N2456	V2291	K2081	T1835	E1645	G1376	ILE	ILE	ILE
ASP	E2865	G2809	Q2748	M2642	L2543	N2456	V2291	K2081	T1835	E1645	G1376	LYS	LYS	LYS
ASP	L2866	L2810	Q2749	N2642	L2543	N2456	V2291	K2081	T1835	E1645	G1376	ALA	ALA	ALA
ASP	A2867	L2811	H2751	M2648	H2549	R2458	L2293	V2082	S1837	M1648	R1386	LEU	LEU	LEU
ASP	T2868	T2812	L2752	T2649	H2549	R2458	L2293	V2082	S1837	M1648	R1386	LYS	LYS	LYS
ASP	Q2879	F2817	L2753	F2650	H2549	R2458	L2293	V2082	S1837	M1648	R1386	GLY	GLY	GLY
ASP	K2880	R2818	V2754	P2756	D2554	D2460	V2302	S2096	K1849	K1652	R1392	ILE	ILE	ILE
ASP	E2881	D2819	K2755	P2756	D2554	D2460	V2302	S2096	K1849	K1652	R1392	ILE	ILE	ILE
ASP	F2882	P2820	D2757	D2757	D2554	D2460	V2302	S2096	K1849	K1652	R1392	ILE	ILE	ILE
ASP	L2884	F2821	D2757	D2757	D2554	D2460	V2302	S2096	K1849	K1652	R1392	ILE	ILE	ILE
ASP	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER
LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	298552	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1100	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	43.996	Depositor
Minimum map value	-17.599	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.916	Depositor
Recommended contour level	3	Depositor
Map size (Å)	378.4, 378.4, 378.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.946, 0.946, 0.946	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0/22775	0.42	0/30861

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	22338	0	22339	488	0
2	A	1	0	0	0	0
All	All	22339	0	22339	488	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 11.

The worst 5 of 488 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:2080:LYS:HG2	1:A:2198:ASN:HD22	1.28	0.95
1:A:3096:PRO:HA	1:A:3099:LEU:HD12	1.57	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3068:ARG:HE	1:A:3075:ALA:HB1	1.40	0.85
1:A:2614:LEU:HD23	1:A:2615:ARG:HH21	1.40	0.84
1:A:545:MET:HE1	1:A:649:MET:HE1	1.59	0.84

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	2791/3223 (87%)	2688 (96%)	102 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	812	ASN

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	2490/2880 (86%)	2479 (100%)	11 (0%)	89 93

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1528	MET
1	A	1764	THR
1	A	2613	VAL
1	A	2541	ILE
1	A	815	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1901	GLN
1	A	3042	GLN
1	A	2164	GLN
1	A	3196	ASN
1	A	2603	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

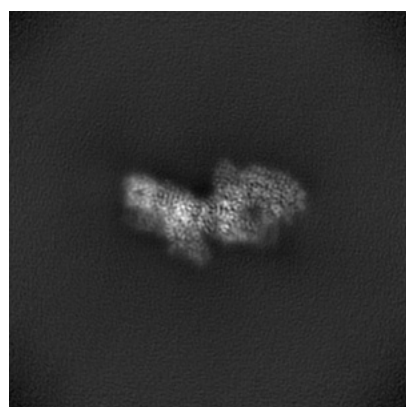
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52990. These allow visual inspection of the internal detail of the map and identification of artifacts.

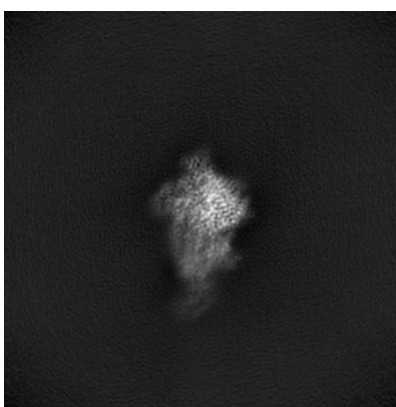
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

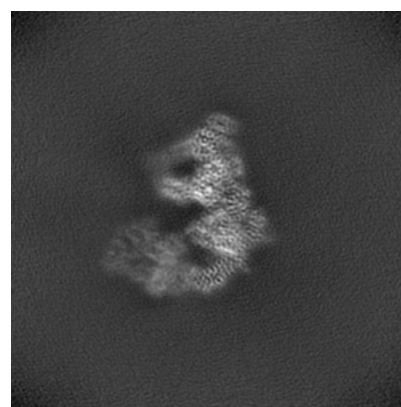
6.1.1 Primary map



X



Y

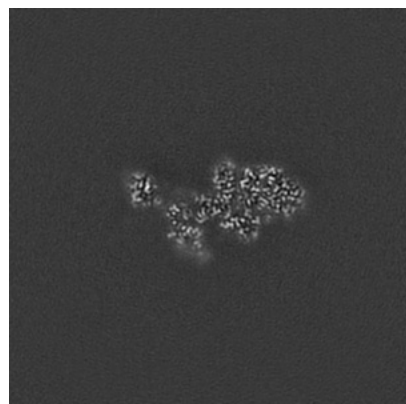


Z

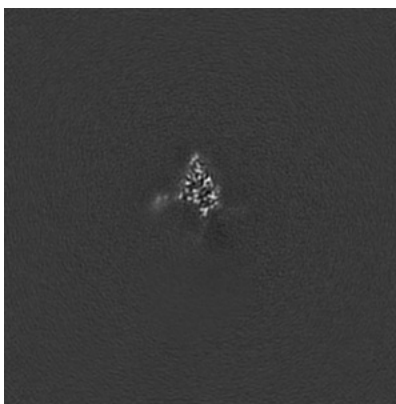
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

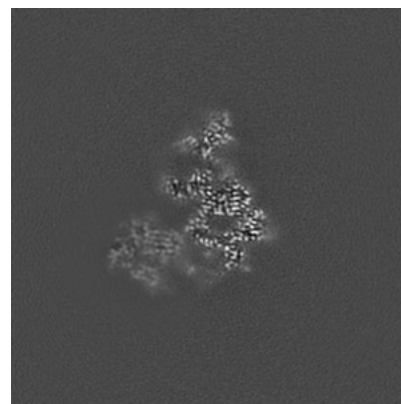
6.2.1 Primary map



X Index: 200



Y Index: 200

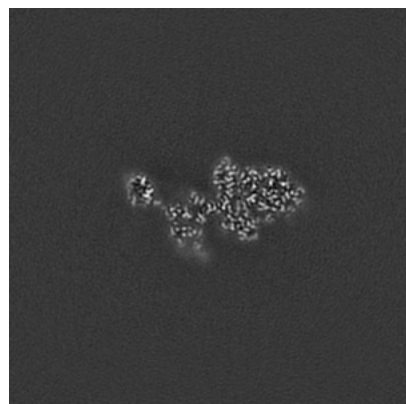


Z Index: 200

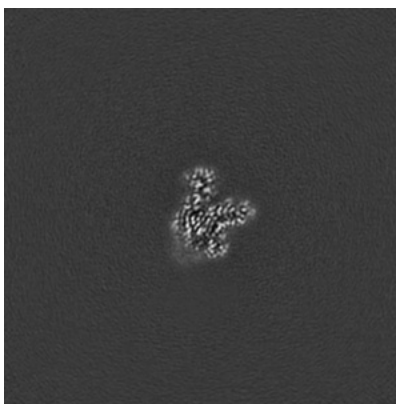
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

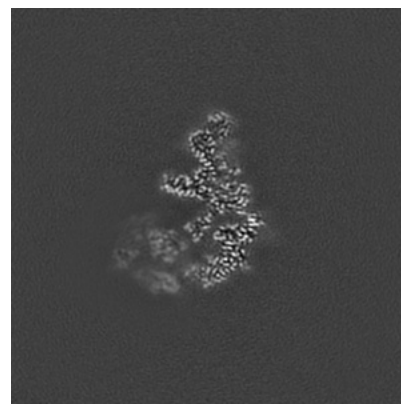
6.3.1 Primary map



X Index: 198



Y Index: 218

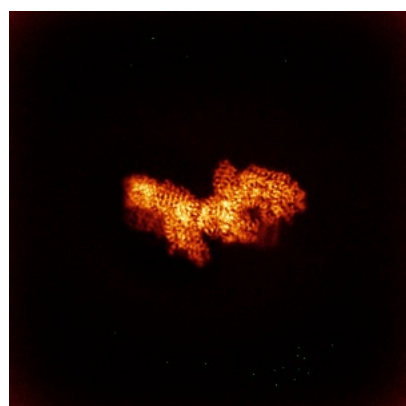


Z Index: 206

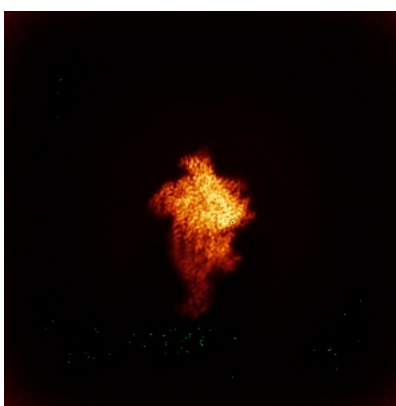
The images above show the largest variance slices of the map in three orthogonal directions.

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

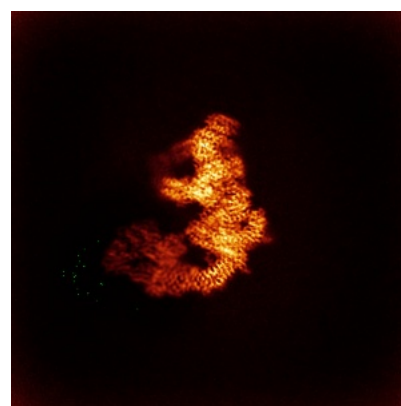
6.4.1 Primary map



X



Y

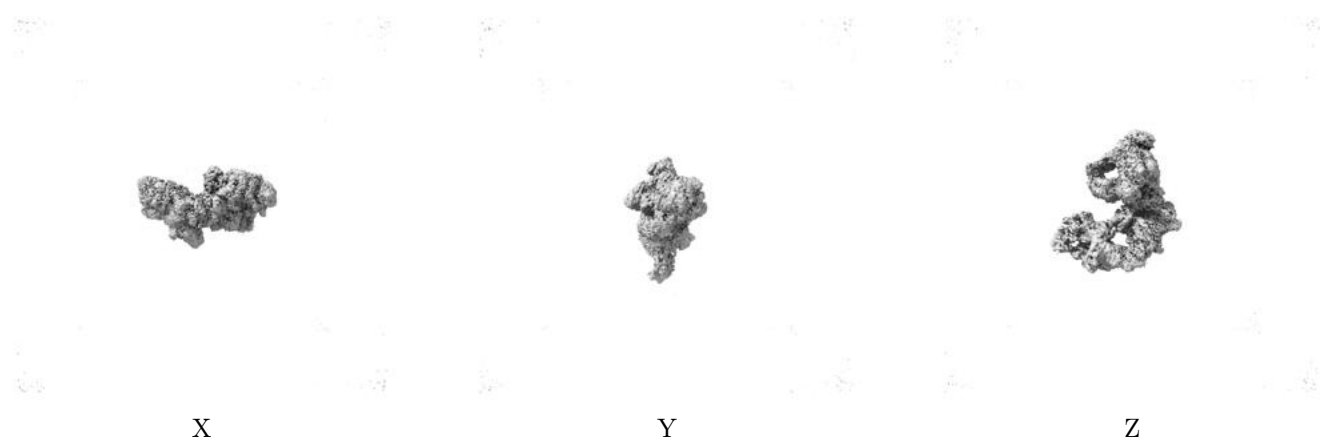


Z

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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

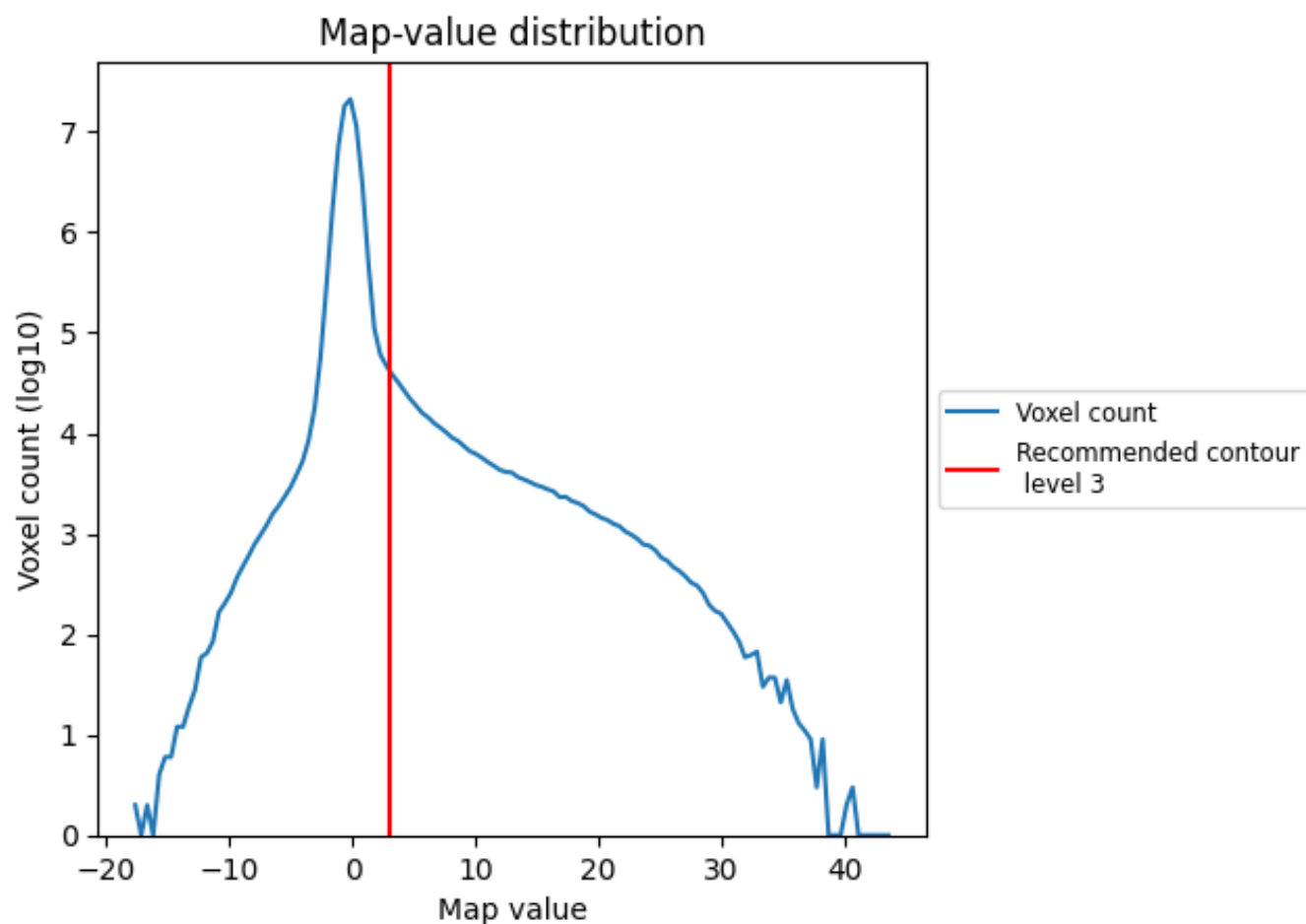
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

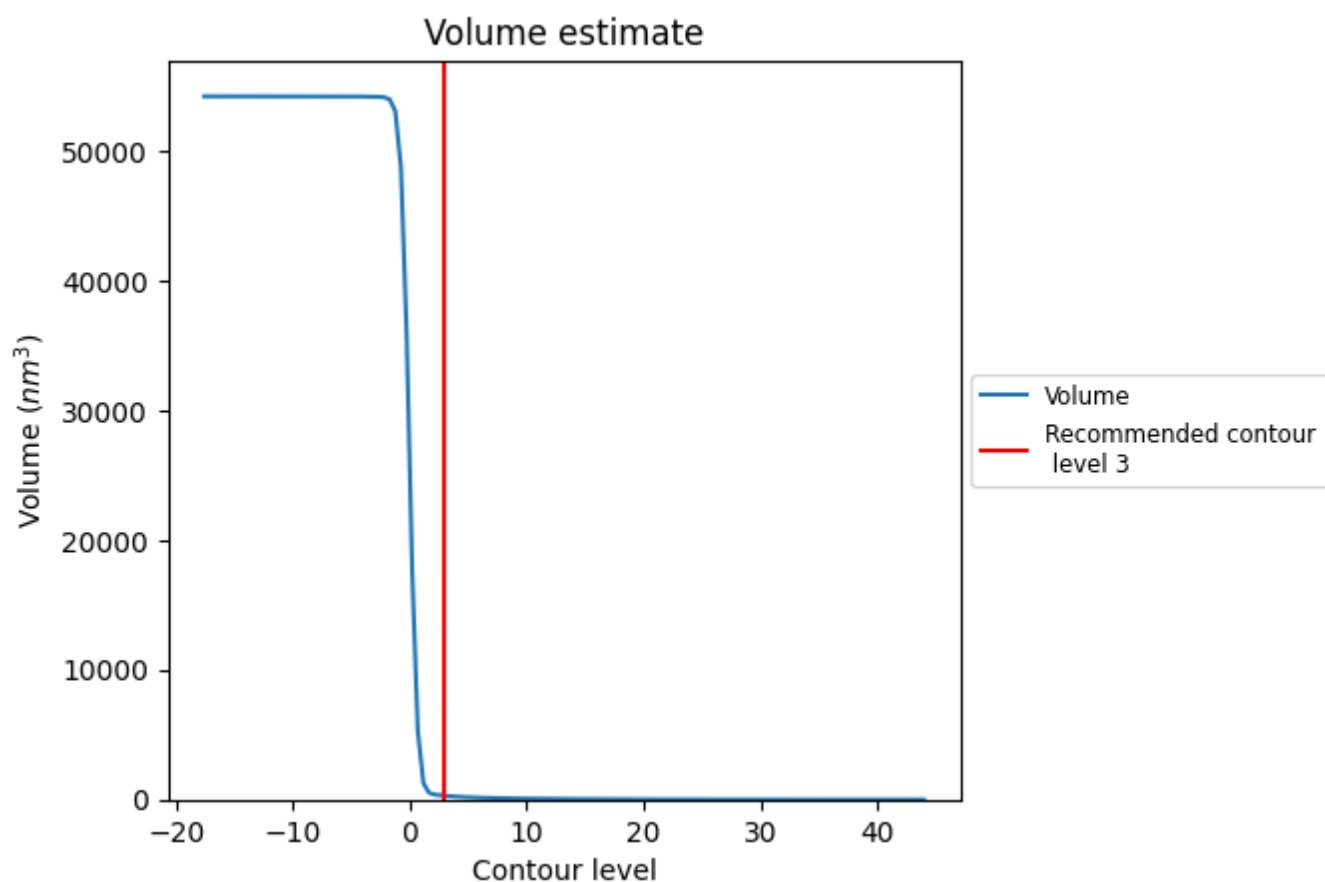
This section contains the results of statistical analysis of the map.

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.

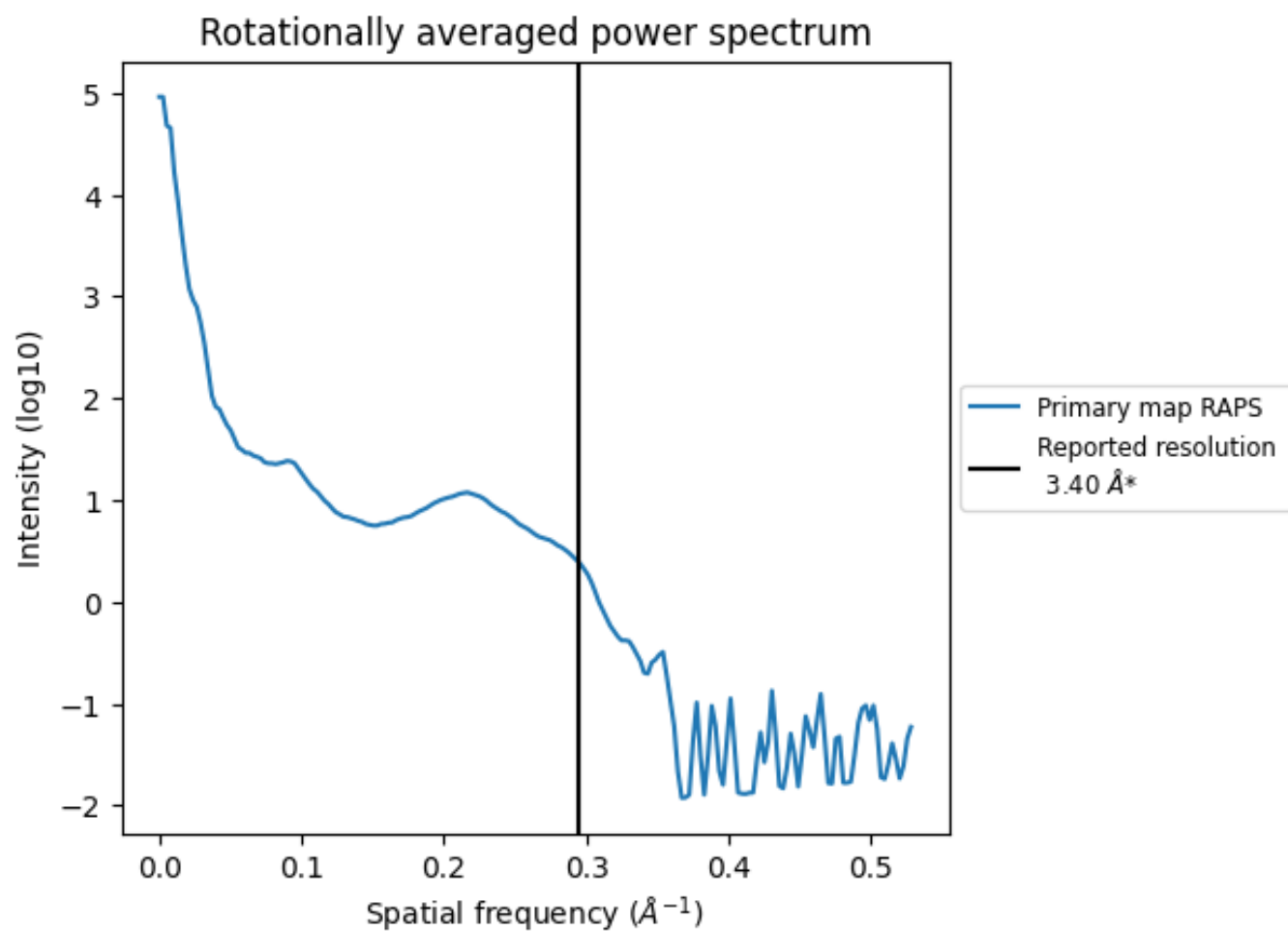
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290 nm^3 ; this corresponds to an approximate mass of 262 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 0.294 Å⁻¹

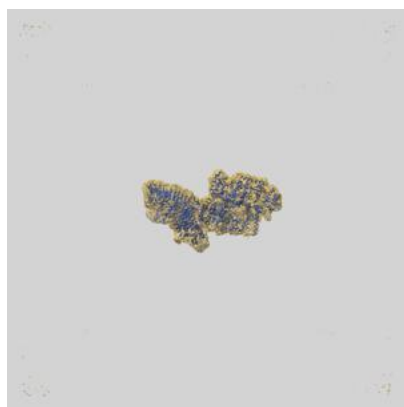
8 Fourier-Shell correlation

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

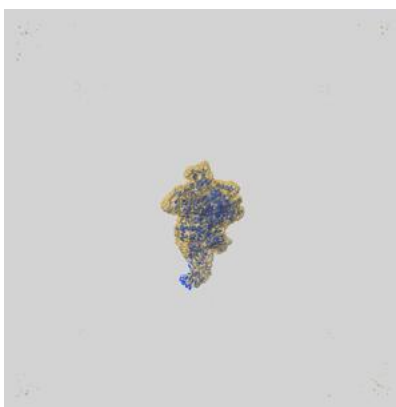
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52990 and PDB model 9QB8. Per-residue inclusion information can be found in section [3](#) on page [4](#).

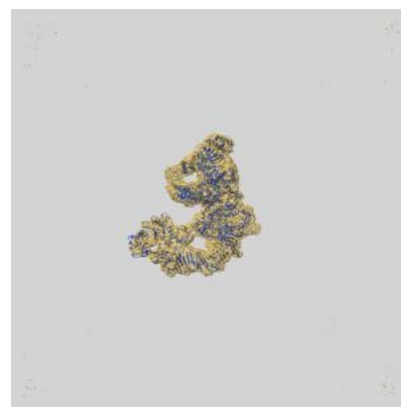
9.1 Map-model overlay [i](#)



X



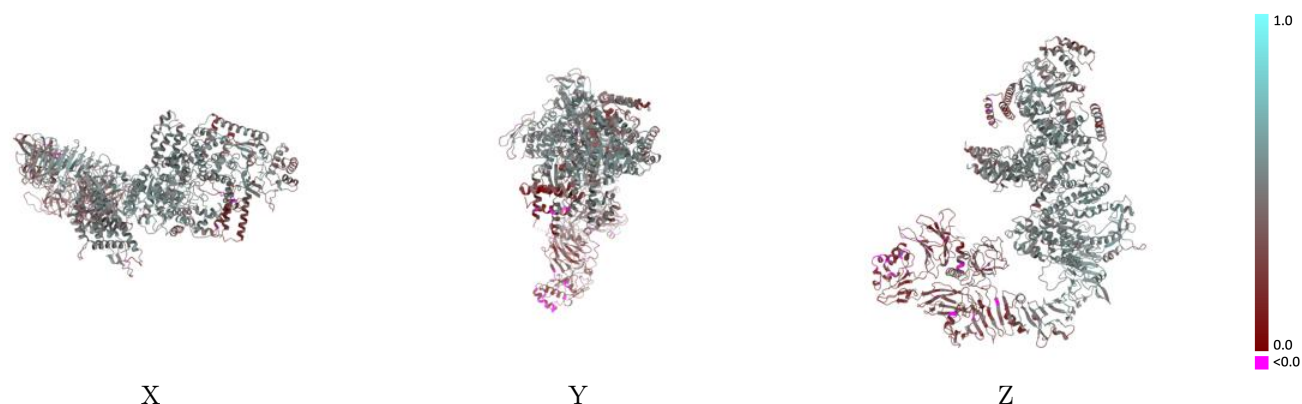
Y



Z

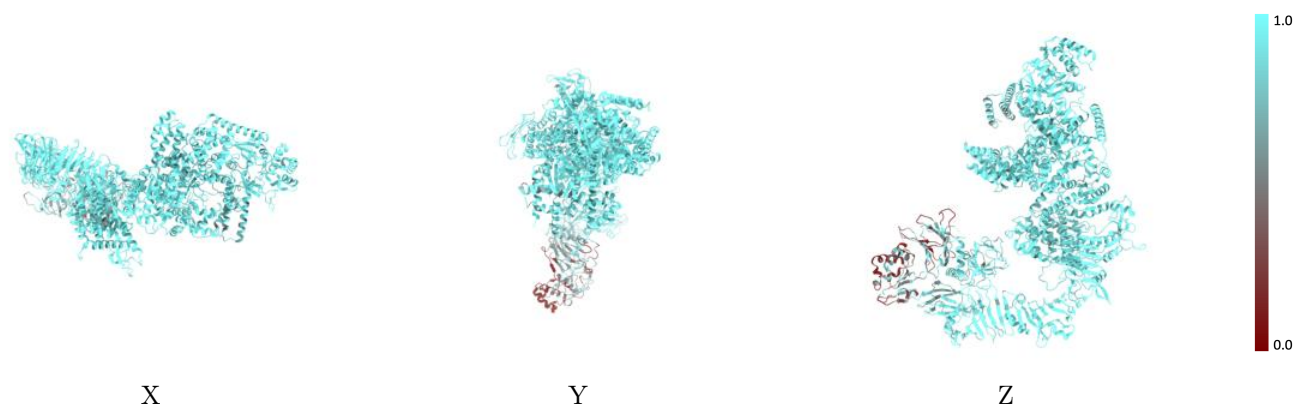
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



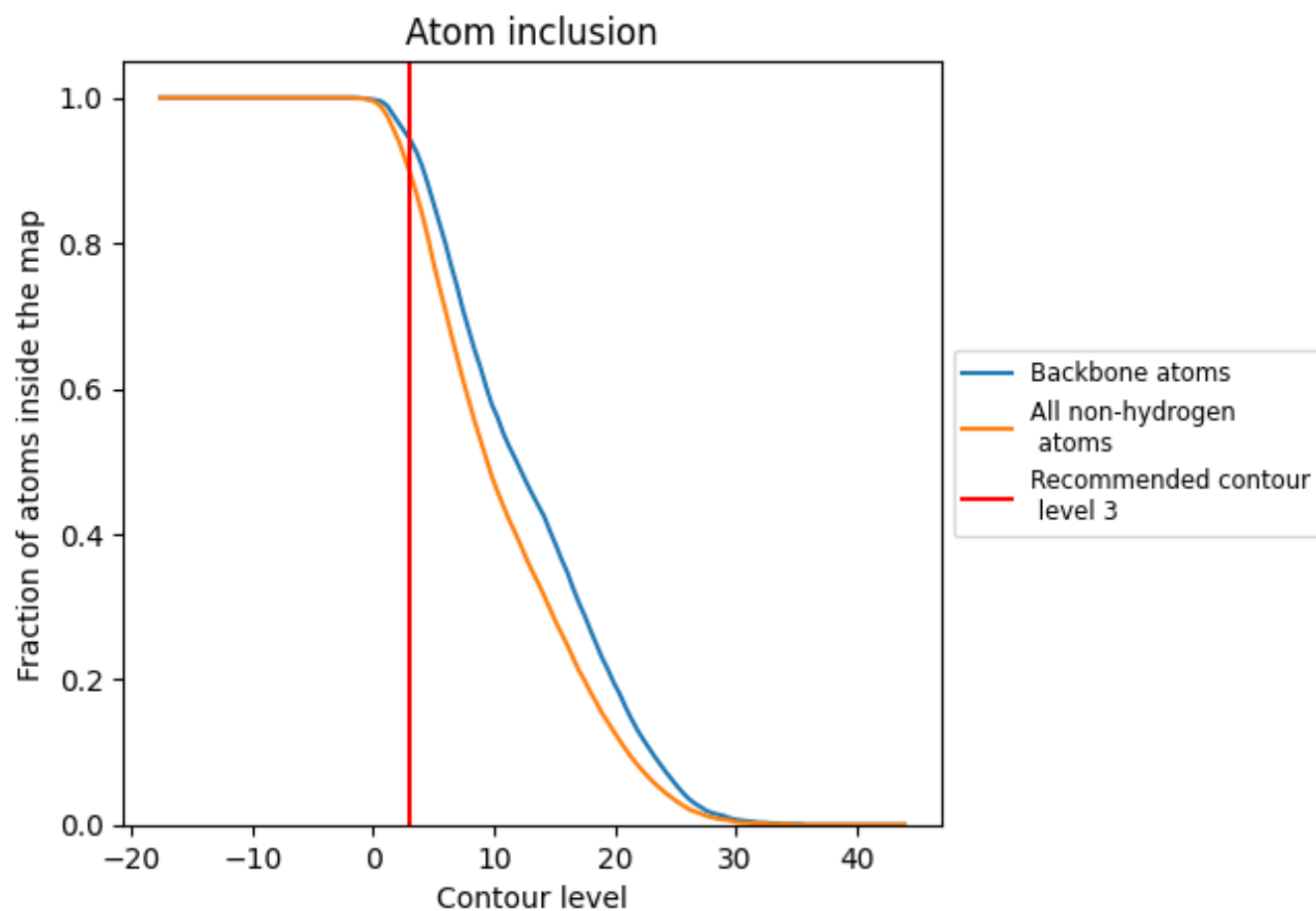
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9000	<div></div> 0.4230
A	<div></div> 0.9000	<div></div> 0.4230

