



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2025 – 02:15 am BST

PDB ID : 9EUW / pdb_00009euw
EMDB ID : EMD-19988
Title : Lymphostatin, conformation 2 (composite structure)
Authors : Griessmann, M.; Rasmussen, T.; Bottcher, B.
Deposited on : 2024-03-28
Resolution : 2.80 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.dev117
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) : 2.42

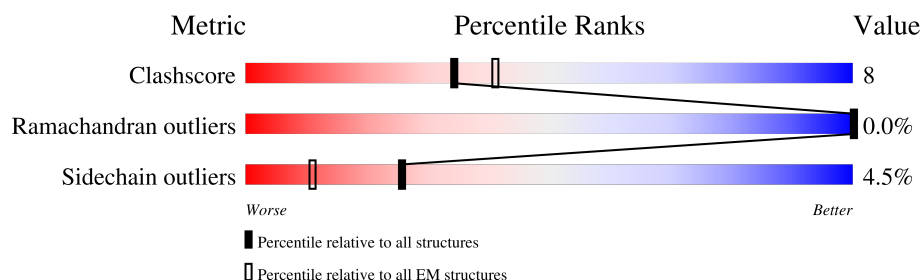
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	3229	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22338 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.

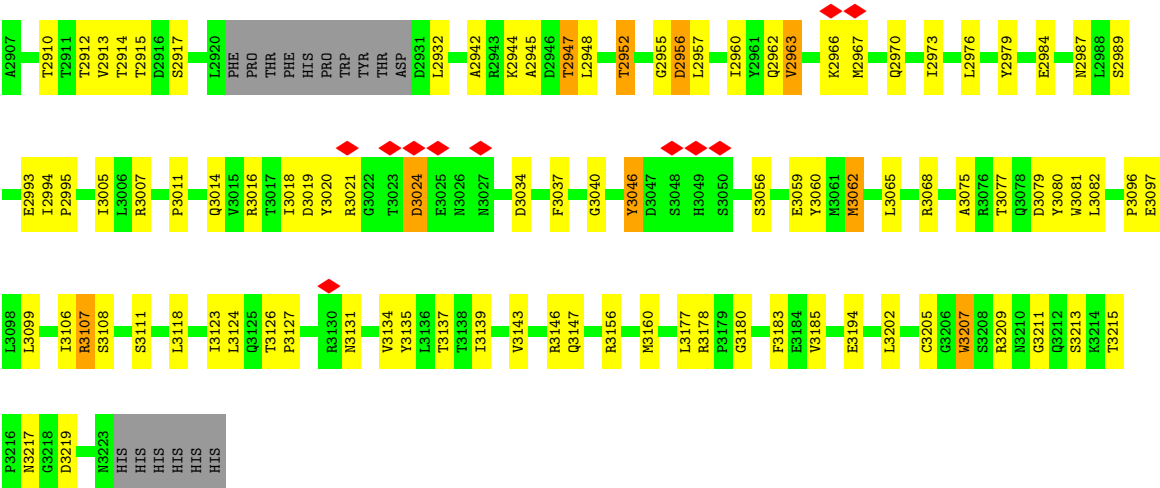
- Molecule 1 is a protein called Efa1/LifA protein.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3224	HIS	-	expression tag	UNP B7UI23
A	3225	HIS	-	expression tag	UNP B7UI23
A	3226	HIS	-	expression tag	UNP B7UI23
A	3227	HIS	-	expression tag	UNP B7UI23
A	3228	HIS	-	expression tag	UNP B7UI23
A	3229	HIS	-	expression tag	UNP B7UI23

E2836	S2742	Q2605	L2473	L2364	W2175	E1988	V1874	R1777	R1573	G1157	LYS
L2837	Q2745	D2606	V2477	N2367	S2187	S2002	R1879	Q1784	S1577	Q1158	GLU
R2838	Q2749	L2610	T2484	S2368	R2188	L2003	L1880	L1340	H1165	ASN	ASN
P2839	Q2750	L2614	Q2485	H2189	H2189	F2012	Q1883	F1797	R1178	THR	THR
L2841	H2751	L2617	R2493	H2371	R2191	F2012	G1884	Q1798	Q1380	GLN	GLN
L2842	V2754	P2618	R2493	L2376	E2207	A2029	G1885	P1801	H1182	ASP	ASP
Q2843	K2755	F2619	L2499	P2376	E2207	L2032	R1885	R1802	G1183	LEU	LEU
Q2844	P2756	N2620	Q2500	E2377	V2212	A2033	L1885	R1802	L1184	SER	SER
T2845	D2757	N2620	A2501	T2378	P2214	L2213	GLU	P1607	E1192	LYS	LYS
T2846	Q2623	Q2623	R2502	T2379	E2207	L2213	ASP	H1358	LEU	GLY	GLY
H2846	Q2623	Q2623	R2502	L2380	E2207	L2213	SER	H1358	LEU	GLN	GLN
R2847	R2628	S2629	Q2507	K2384	D2220	N2035	THR	T1364	H210	LEU	LEU
F2848	S2629	G2630	H2513	L2393	T2226	N2035	LEU	I1365	Y1211	SER	SER
L2849	Q2630	Q2630	T2516	L2393	T2226	N2035	ALA	A1366	N1212	LEU	LEU
N2850	V2635	V2635	T2516	L2393	T2226	N2035	LYS	A1366	N1212	GLN	GLN
K2851	M2642	A2643	G2520	N2399	T2226	N2035	ILE	A1367	E1213	LEU	LEU
A2852	L2644	Q2403	S2524	L2400	T2226	N2035	ASN	A1368	D1214	ILE	ILE
L2857	N2648	P2404	Y2526	L2400	T2226	N2035	LEU	T1369	K1231	LYS	LYS
N2867	L2651	D2406	M2529	L2400	T2226	N2035	ALA	L1372	E1232	ALA	ALA
L2868	L2651	L2407	M2529	L2400	T2226	N2035	M1897	R1386	S1233	LYS	LYS
A2869	Q2660	A2408	V2532	L2400	T2226	N2035	D1898	S1401	P1237	GLU	GLU
L2870	Q2660	A2408	V2532	L2400	T2226	N2035	Q1901	M1408	P1248	LEU	LEU
T2871	L2662	L2409	T2533	L2400	T2226	N2035	L1902	F1409	E1251	GLY	GLY
K2873	E2675	N2411	T2639	L2400	T2226	N2035	T1906	K1410	P1255	THR	THR
E2874	L2678	N2411	T2639	L2400	T2226	N2035	M1910	D1416	V1261	LYS	LYS
R2877	L2678	N2411	T2639	L2400	T2226	N2035	I1911	S1427	M1266	THR	THR
Q2879	L2678	N2411	T2639	L2400	T2226	N2035	T1921	F1430	S1282	ASP	ASP
T2880	L2678	N2411	T2639	L2400	T2226	N2035	E1922	E1433	S1292	LEU	LEU
E2881	L2678	N2411	T2639	L2400	T2226	N2035	L1928	R1447	D1301	ASP	ASP
T2884	L2678	N2411	T2639	L2400	T2226	N2035	L1929	D1466	V1307	LYS	LYS
SER	L2678	N2411	T2639	L2400	T2226	N2035	E1930	D1466	V1307	ILE	ILE
LYS	L2678	N2411	T2639	L2400	T2226	N2035	S1931	R1479	R1310	GLU	GLU
ILE	L2678	N2411	T2639	L2400	T2226	N2035	R1943	L1488	N1315	ALA	ALA
LEU	L2678	N2411	T2639	L2400	T2226	N2035	A1956	Q1489	N1315	VAL	VAL
TYR	L2678	N2411	T2639	L2400	T2226	N2035	L1959	D1492	N1318	LYS	LYS
GLN	L2678	N2411	T2639	L2400	T2226	N2035	E1960	D1492	N1318	ASN	ASN
GLY	L2678	N2411	T2639	L2400	T2226	N2035	V1963	M1528	Q1321	LYS	LYS
ALA	L2678	N2411	T2639	L2400	T2226	N2035	L1964	T1547	L1322	HIS	HIS
MET	L2678	N2411	T2639	L2400	T2226	N2035	E1965	H1563	L1322	GLU	GLU
LYS	L2678	N2411	T2639	L2400	T2226	N2035	V1963	H1563	L1322	LEU	LEU
LYS	L2678	N2411	T2639	L2400	T2226	N2035	E1965	H1563	L1322	TYR	TYR
THR	L2678	N2411	T2639	L2400	T2226	N2035	I1978	N1558	K1326	PHE	PHE
ASP	L2678	N2411	T2639	L2400	T2226	N2035	Q1981	N1558	K1326	GLU	GLU
GLY	L2678	N2411	T2639	L2400	T2226	N2035	Q1982	N1558	K1326	LYS	LYS
PRO	L2678	N2411	T2639	L2400	T2226	N2035	A1983	N1558	K1326	ILE	ILE
VAL	L2678	N2411	T2639	L2400	T2226	N2035	T1984	N1558	K1326	LYS	LYS
VAL	L2678	N2411	T2639	L2400	T2226	N2035	T1984	N1558	K1326	LYS	LYS
GLU	L2678	N2411	T2639	L2400	T2226	N2035	T1984	N1558	K1326	LYS	LYS
ASP	L2678	N2411	T2639	L2400	T2226	N2035	T1984	N1558	K1326	LYS	LYS



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	182000	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	68.256	Depositor
Minimum map value	-34.889	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	1.109	Depositor
Recommended contour level	6.5	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](#)

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	0.27	0/22775	0.49	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	22342	354	0
All	All	22338	0	22342	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 8.

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:A:1857:LEU:HB3	1:A:1943:ARG:HH12	1.43	0.83
1:A:1853:MET:O	1:A:1857:LEU:HB2	1.84	0.77
1:A:1812:ASN:HB3	1:A:1826:GLN:H	1.51	0.75
1:A:2380:LEU:HD22	1:A:2425:MET:HG3	1.67	0.75
1:A:1683:ALA:HB2	1:A:1746:THR:HG21	1.69	0.75

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	2791/3229 (86%)	2708 (97%)	82 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2187	SER

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	2490/2885 (86%)	2379 (96%)	111 (4%)	23	55

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1866	ASP
1	A	3207	TRP
1	A	2524	SER
1	A	3205	CYS
1	A	2967	MET

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	271	GLN
1	A	1350	GLN
1	A	1358	HIS
1	A	1901	GLN
1	A	2106	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

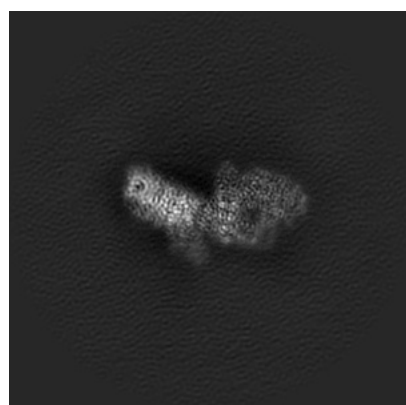
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19988. These allow visual inspection of the internal detail of the map and identification of artifacts.

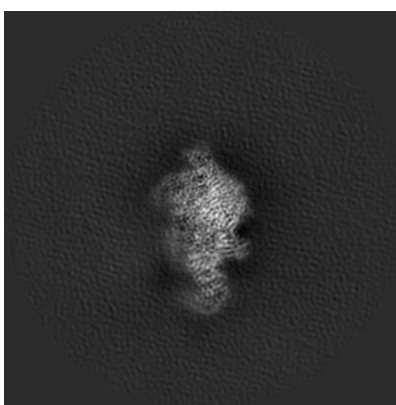
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

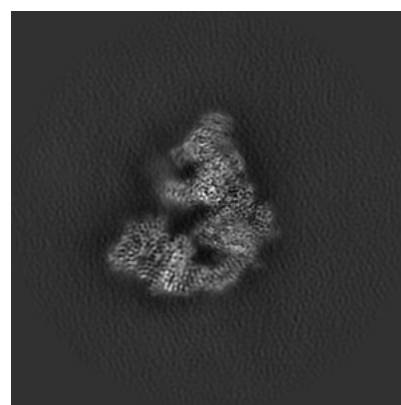
6.1.1 Primary map



X



Y

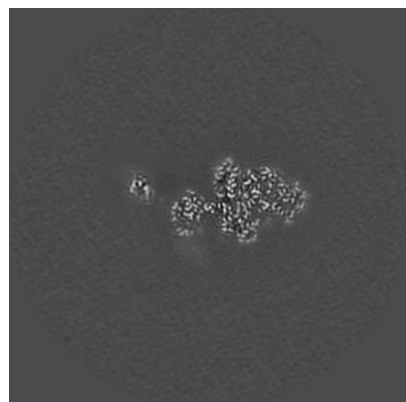


Z

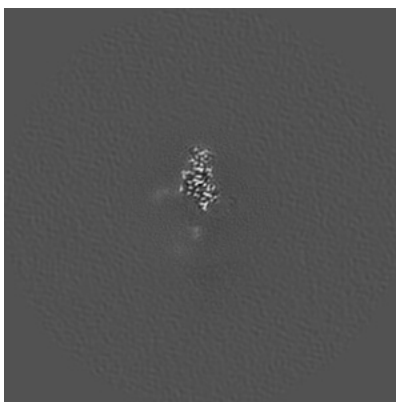
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

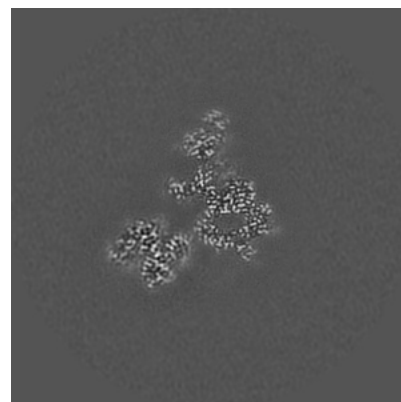
6.2.1 Primary map



X Index: 200



Y Index: 200

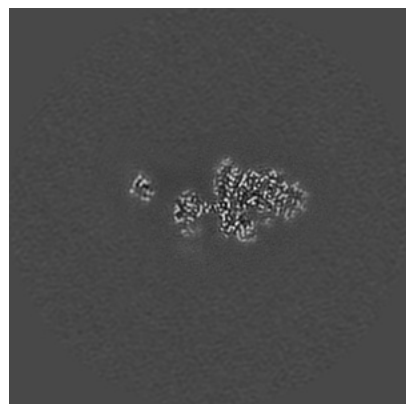


Z Index: 200

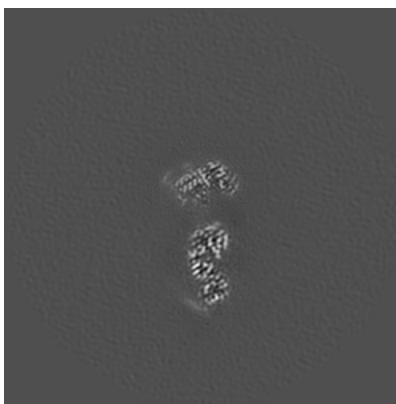
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

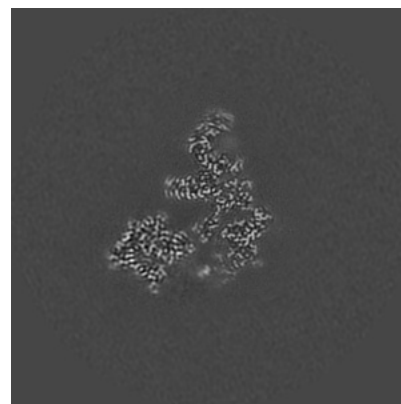
6.3.1 Primary map



X Index: 198



Y Index: 161

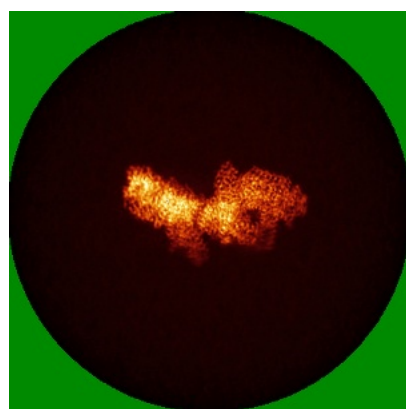


Z Index: 207

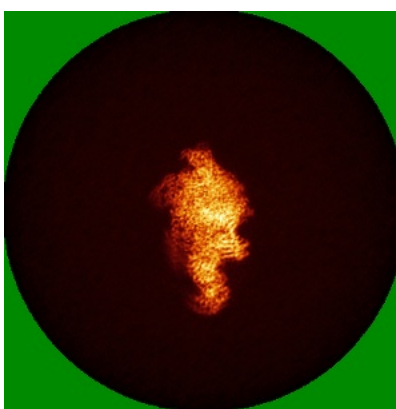
The images above show the largest variance slices of the map in three orthogonal directions.

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

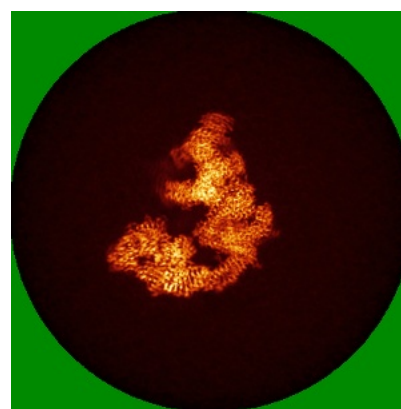
6.4.1 Primary map



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

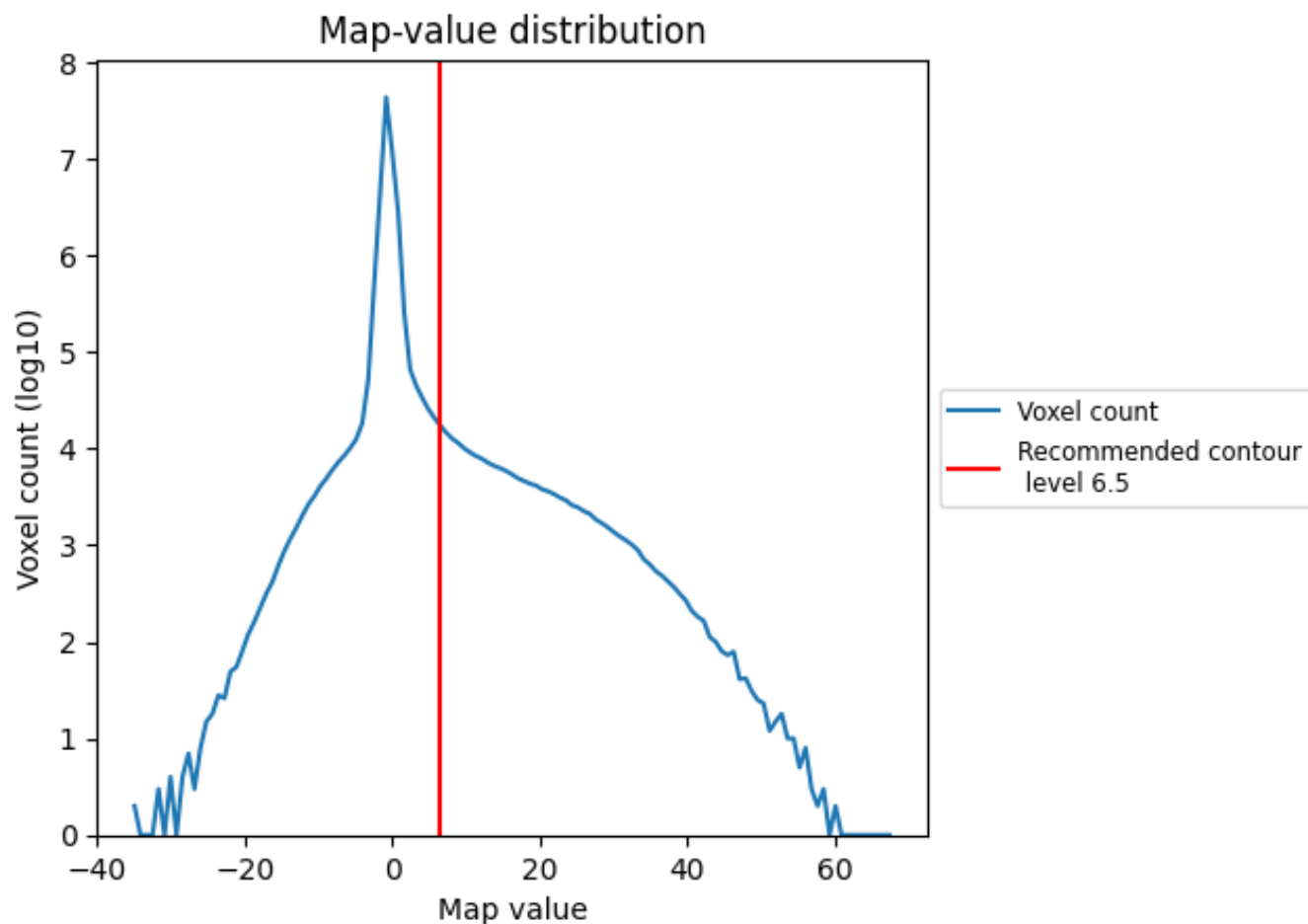
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

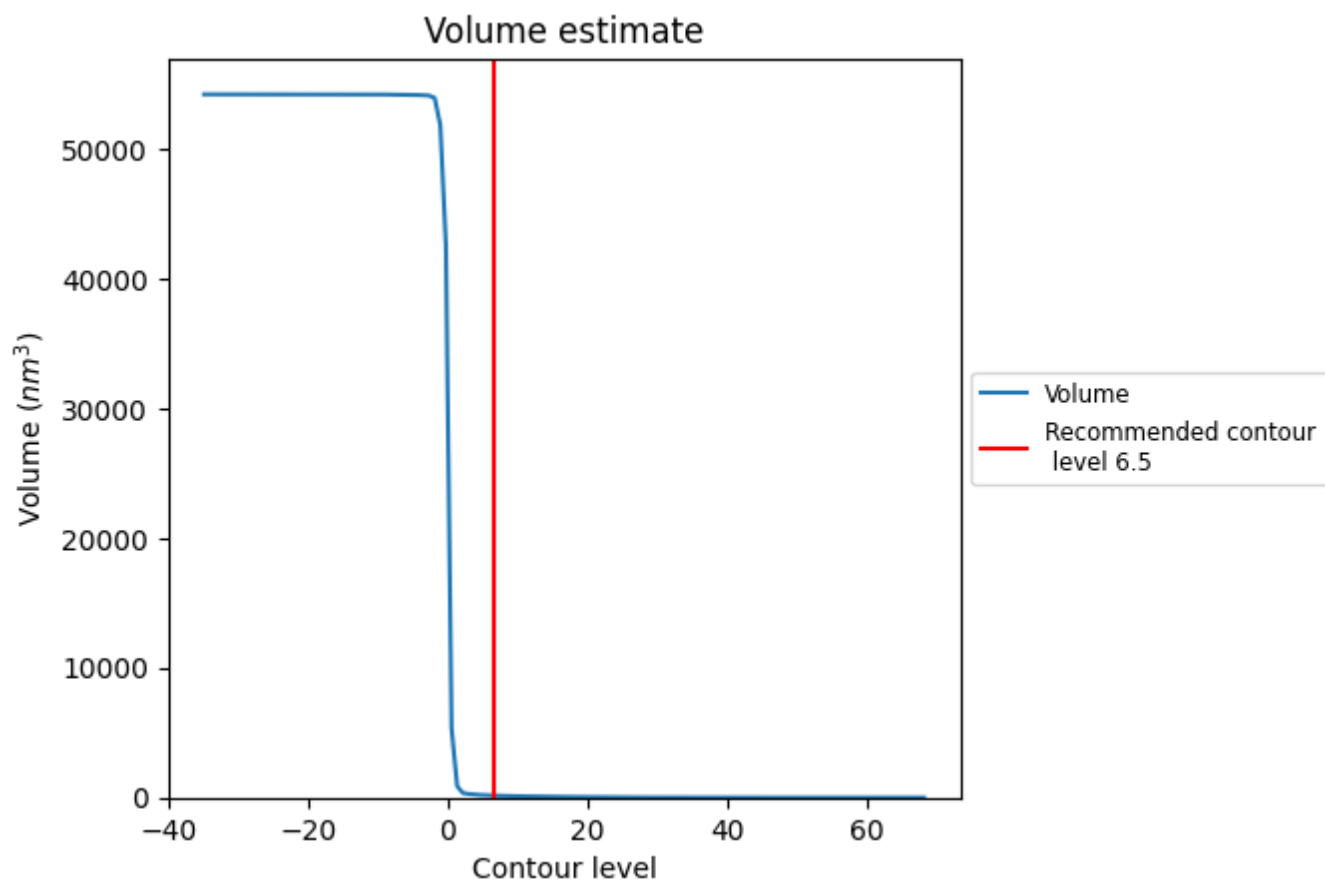
This section contains the results of statistical analysis of the map.

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.

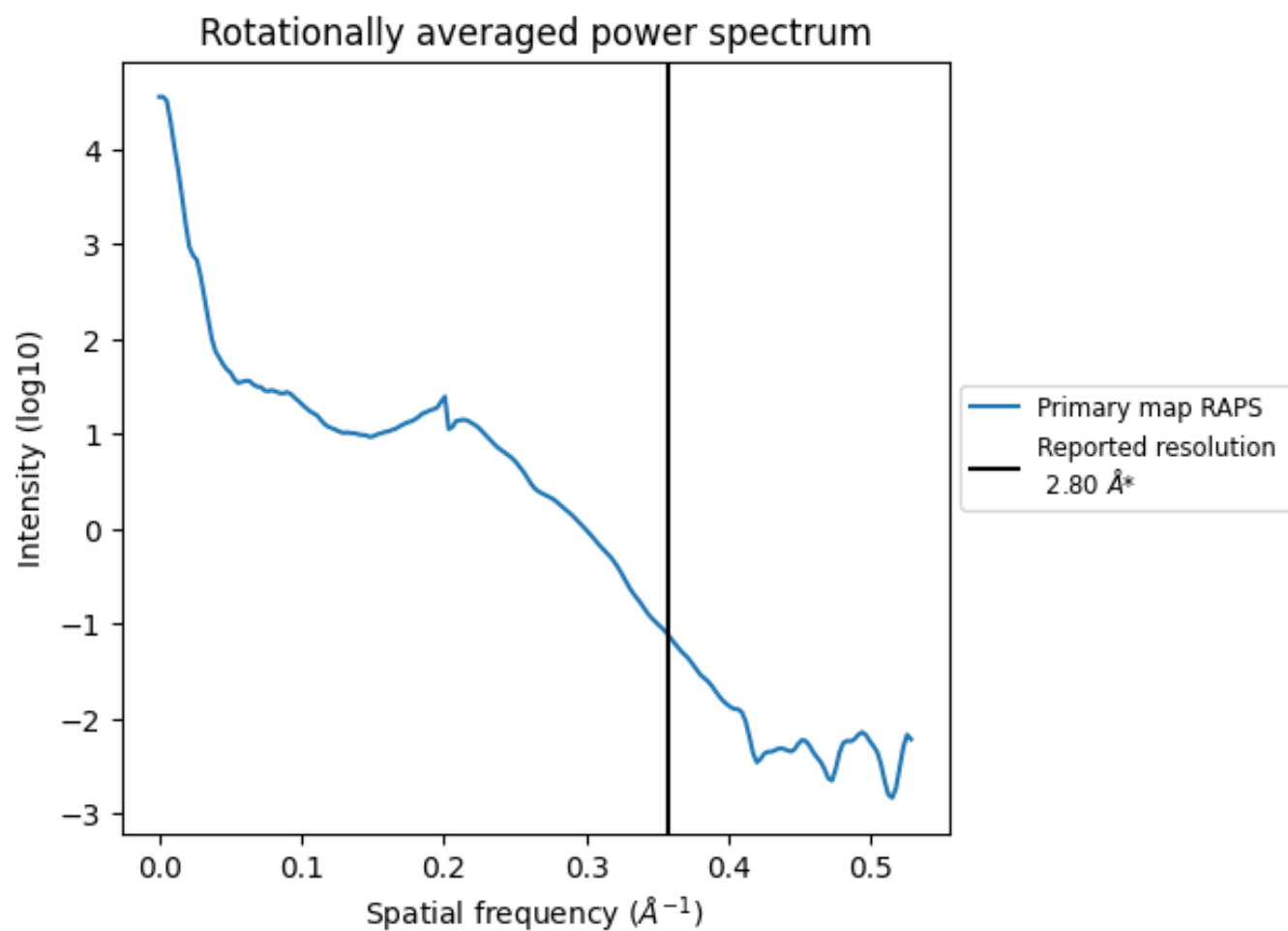
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 156 nm^3 ; this corresponds to an approximate mass of 141 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 0.357 Å⁻¹

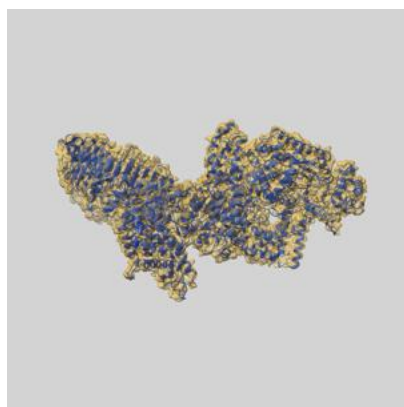
8 Fourier-Shell correlation ⓘ

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

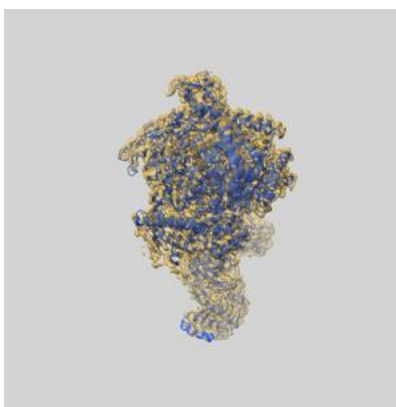
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19988 and PDB model 9EUW. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

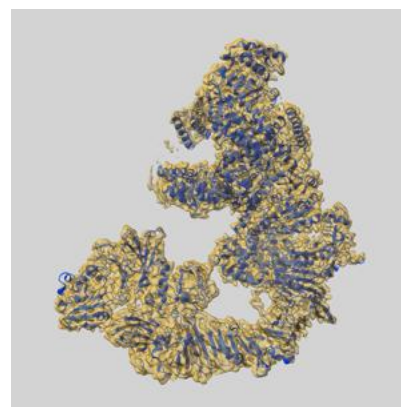
9.1 Map-model overlay [i](#)



X



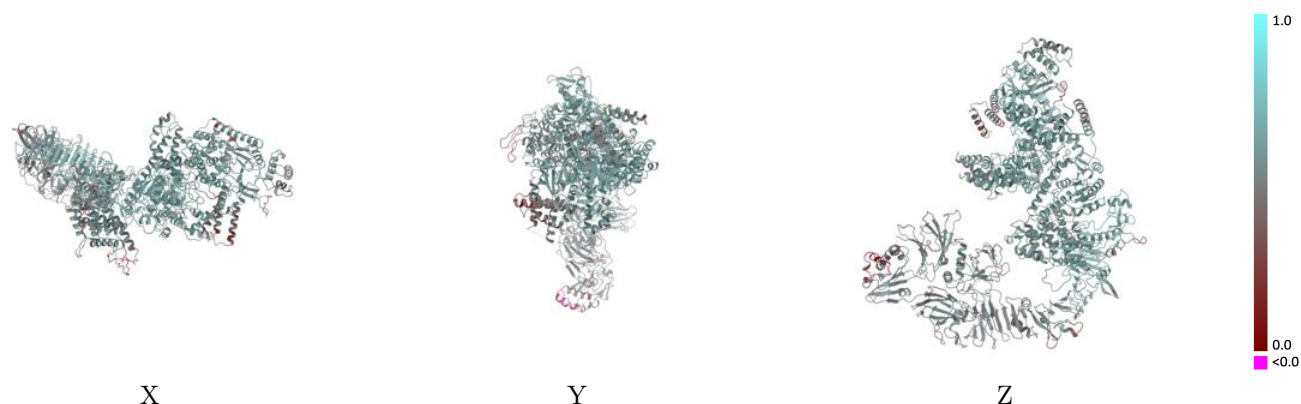
Y



Z

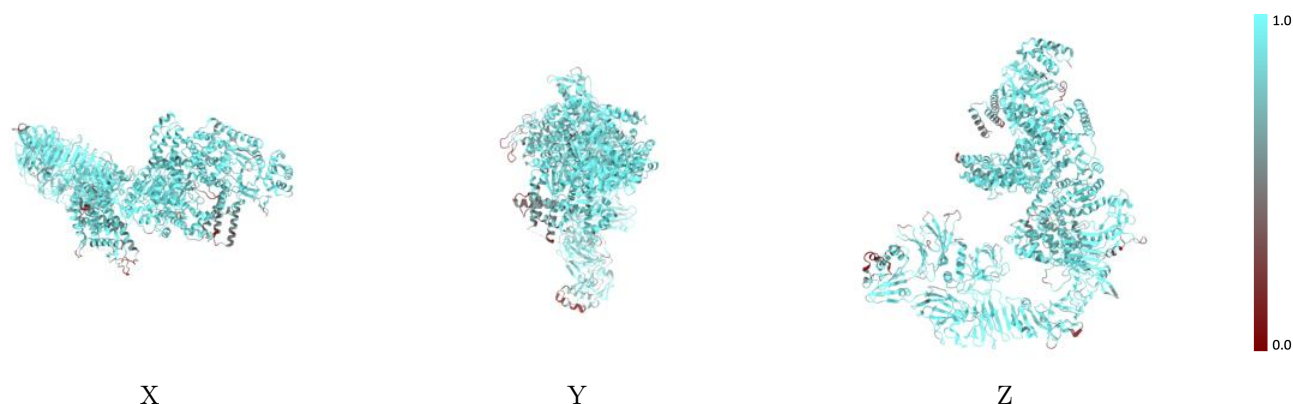
The images above show the 3D surface view of the map at the recommended contour level 6.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



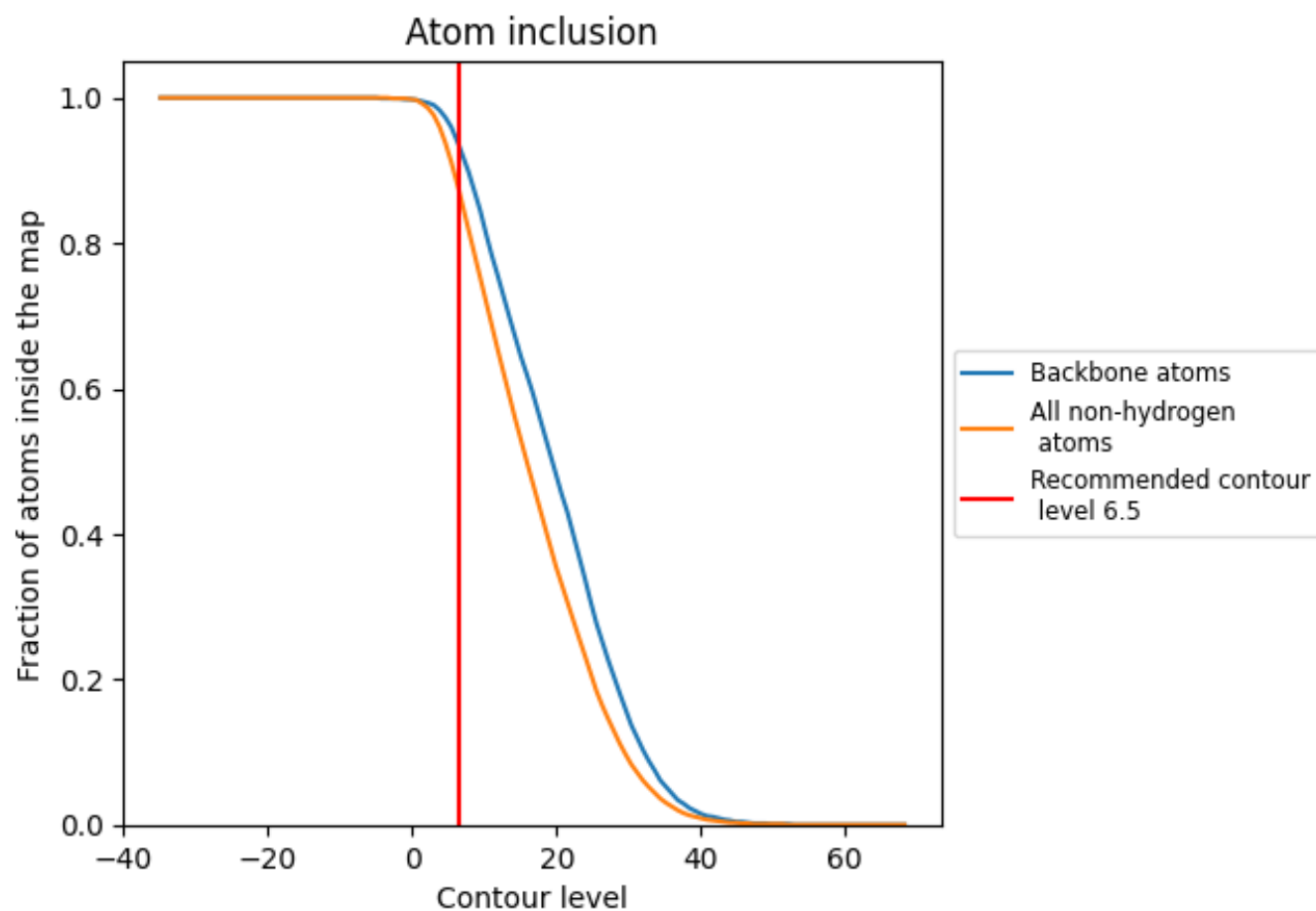
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% 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 (6.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8720	<div><div></div></div> 0.5430
A	<div><div></div></div> 0.8720	<div><div></div></div> 0.5430

