



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:58 PM UTC

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:

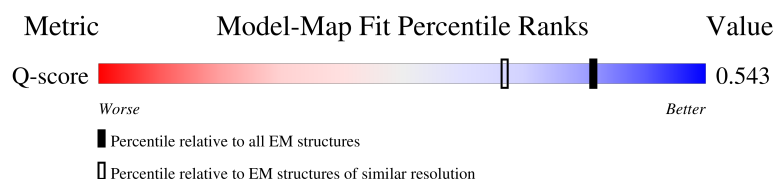
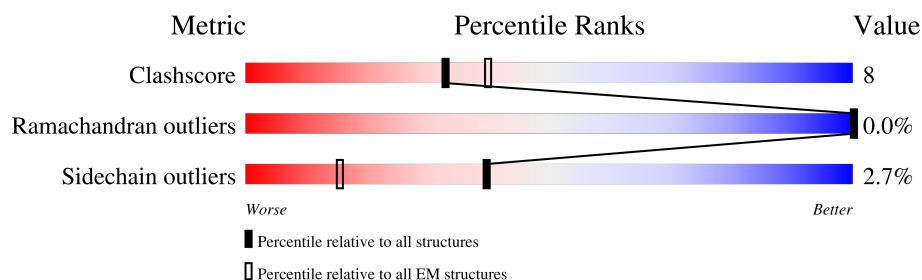
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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.

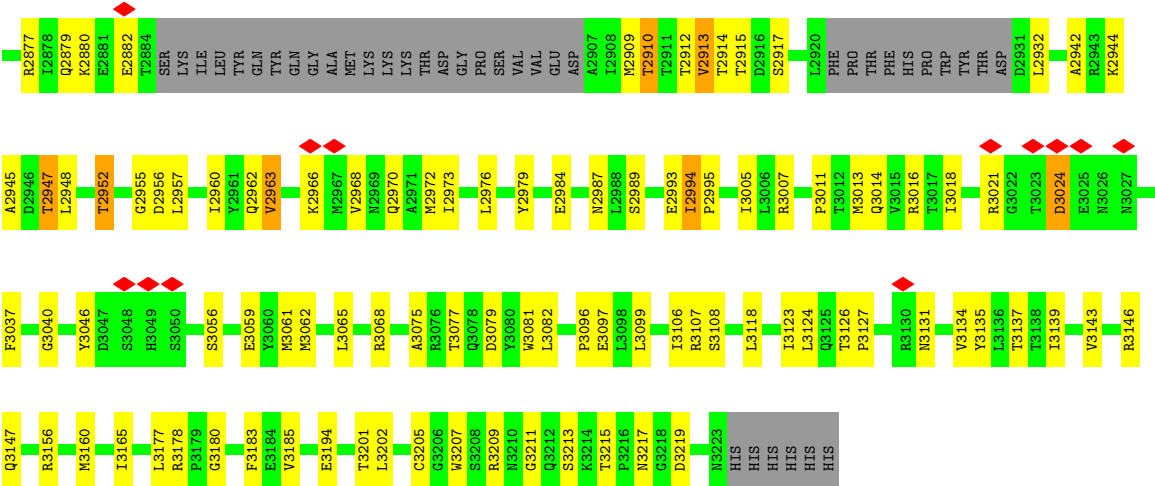
- Molecule 1 is a protein called Efa1/LifA protein.

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

R2795	R2805	R2814	R2815	R2816	R2817	R2818	R2819	R2820	R2821	R2822	R2823	R2824	R2825	R2826	R2827	R2828	R2829	R2830	R2831	R2832	R2833	R2834	R2835	R2836	R2837	R2838	R2839	R2840	R2841	R2842	R2843	R2844	R2845	R2846	R2847	R2848	R2849	R2850	R2851	R2852	R2853		R2857	R2867	R2868	R2869	R2870	R2871	R2872	A2874
Q2645	Q2646	Q2647	Q2648	L2651	Q2660	V2661	L2662	L2678	K2682	A2689	F2689	F2692	N2698	I2699	L2702	S2708	I2713	V2720	E2731	L2732	L2733	L2734	L2735	L2736	L2737	L2738	L2739	S2742	Q2745	Q2749	E2750	H2751	L2752	L2753	L2754	L2755	L2756	L2757	L2773	L2781	K2782	L2783		R2791	L2792	L2793	R2794			
T2516	G2520	R2525	Y2526	M2529	V2532	T2533	T2539	L2543	A2544	G2545	G2546	H2547	H2548	H2549	P2550	E2551	T2552	L2553	D2554	E2564	A2577	S2582	S2588	G2589	L2594	Q2603	P2604	Q2605	D2606	L2610	D2619	N2620	V2623	R2628	S2629	G2630	V2635	M2642	A2643	L2644										
L2393	N2399	L2400	N2401	V2402	Q2403	P2404	E2405	D2406	E2407	K2408	L2410	G2415	R2418	D2423	G2424	M2425	A2429	R2432	E2433	N2434	G2435	L2440	V2451	D2460	A2461	D2464	R2465	L2466	S2472	L2473	V2477	T2484	Q2485	R2493	L2499	Q2500	A2501	R2502	Q2507	H2513										
L2221	T2226	I2230	T2268	L2269	S2270	D2283	L2284	S2285	V2291	M2292	L2293	K2294	T2295	P2296	D2297	V2302	M2303	T2304	I2305	T2312	L2313	V2314	A2318	D2327	T2331	G2345	R2354	D2355	L2356	K2357	L2364	S2365	S2366	N2367	S2368	H2371	L2375	P2376	E2377	T2378	T2379	L2380	K2384							
K2033	R2034	N2035	V2036	K2037	L2038	K2039	E2040	E2041	R2042	L2043	T2044	Q2045	I2060	F2078	G2079	K2080	L2091	E2095	D2101	R2102	H2106	R2107	P2108	D2109	R2116	V2119	A2122	Y2135	K2139	D2153	N2174	K2175	S2187	R2188	H2189	K2190	R2191	E2207	V2212	L2213	P2214	D2220								
LEU	ALA	LYS	ILE	ASN	LEU	ALA	M1897	L1898	Q1901	L1902	T1906	M1910	F1823	F1824	F1825	Q1826	D1829	G1830	E1831	T1832	L1833	H1834	T1835	T1836	V1837	V1838	E1839	E1842	Q1848	K1849	L1850	S1851	T1852	M1853	L1854	L1857	P1858	A1859	G1861	I1862	V1874	R1879	L1880	G1883	G1884	H1885	GLU	ASP	SER	THR
R1806	H1807	L1808	V1810	E1811	I1812	I1813	E1814	L1815	A1816	D1817	R1822	F1823	N1824	L1825	Q1826	D1829	G1830	E1831	T1832	L1833	H1834	T1835	T1836	V1837	V1838	E1839	E1842	Q1848	K1849	L1850	S1851	T1852	M1853	L1854	L1857	P1858	A1859	G1861	I1862	V1874	R1879	L1880	G1883	G1884	H1885	GLU	ASP	SER	THR	
T1623	L1631	I1635	E1645	S1646	M1648	L1654	T1670	A1674	E1678	A1683	V1689	K1690	D1694	I1695	L1716	Q1736	A1737	D1738	M1739	I1740	R1741	T1746	Q1747	I1749	R1754	M1760	T1773	R1777	Q1784	F1797	Q1798	P1801	R1802	S1803	S1804	G1805														
T1364	I1365	D1367	A1368	T1369	L1372	R1386	S1401	M1408	F1409	K1410	D1416	S1427	F1430	E1433	R1447	R1479	L1488	Q1489	T1547	H1553	N1558	Q1559	T1562	T1563	E1573	S1577	T1578	Y1592	R1593	L1594	P1607	A1610	I1614	E1615	I1618	Q1619														
H1210	Y1211	N1212	E1213	D1214	S1233	S1234	I1235	P1237	P1248	E1251	P1255	V1261	M1266	S1282	S1292	D1301	V1307	R1309	R1310	N1315	S1316	Q1317	N1318	Q1321	L1322	L1323	E1324	N1325	S1326	V1327	S1328	L1332	S1336	L1340	Q1350	H1356	Q1357	H1358												
SER	THR	LYS	GLU	GLN	LYS	LEU	GLN	SER	GLN	ALA	ASN	GLU	PHE	LEU	GLY	ILE	SER	THR	PHE	ILE	LYS	TYR	GLU	ARG	LEU	LEU	ASP	A1119	F1120	F1121	K1122	K1136	E1141	Y1142	S1143	R1144	I1147	D1151	K1152	V1153	I1154	F1155	Q1158	R1178	H1182	G1183	L1184	E1192		
MET	LYS	ASP	HIS	LEU	SER	LEU	GLN	SER	GLN	ALA	ASN	GLU	PHE	LEU	GLY	ILE	SER	THR	PHE	ILE	LYS	TYR	GLU	ARG	LEU	LEU	ASP	A1119	F1120	F1121	K1122	K1136	E1141	Y1142	S1143	R1144	I1147	D1151	K1152	V1153	I1154	F1155	Q1158	R1178	H1182	G1183	L1184	E1192		



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 ($\text{\AA}$)	378.4, 378.4, 378.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.19	0/22775	0.32	2/30861 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2188	ARG	CB-CA-C	-5.24	110.51	116.54
1	A	2647	VAL	N-CA-C	-5.02	108.38	113.20

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	373	0
All	All	22338	0	22342	373	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 373 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	2423 (97%)	67 (3%)	39	74

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2947	THR
1	A	2963	VAL
1	A	3165	ILE
1	A	1235	SER
1	A	1233	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3014	GLN
1	A	3039	ASN
1	A	3223	ASN
1	A	1278	GLN
1	A	1242	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.

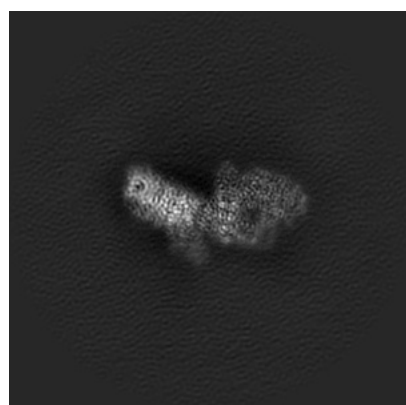
6 Map visualisation [i](#)

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

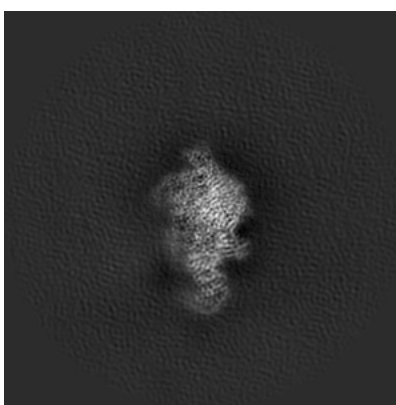
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

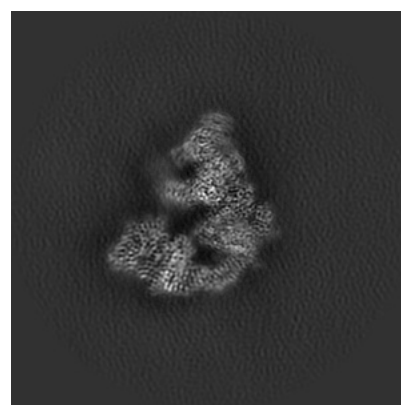
6.1.1 Primary map



X



Y

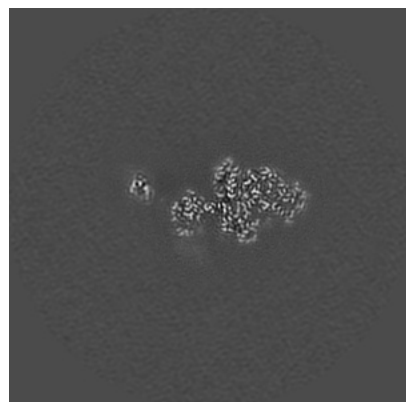


Z

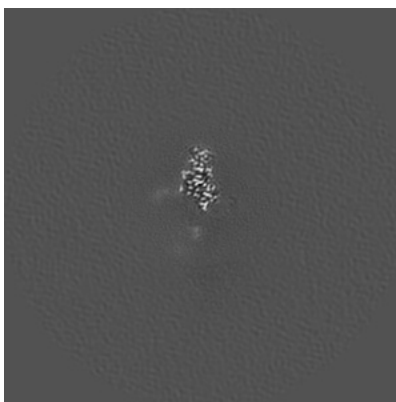
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

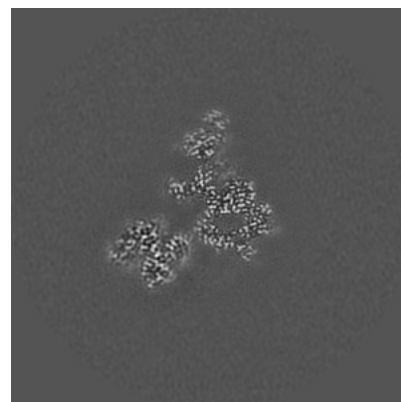
6.2.1 Primary map



X Index: 200



Y Index: 200

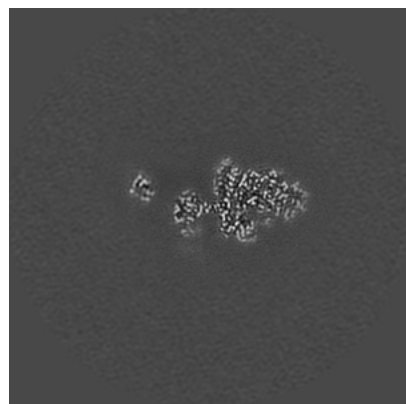


Z Index: 200

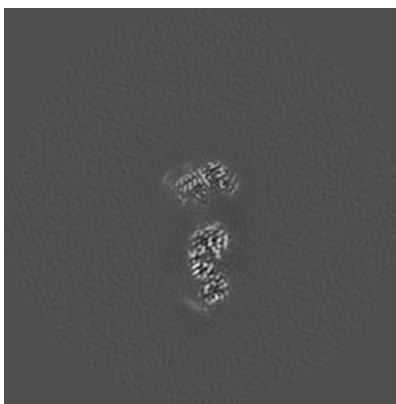
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

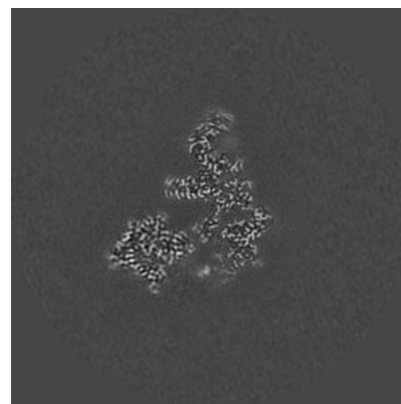
6.3.1 Primary map



X Index: 198



Y Index: 161

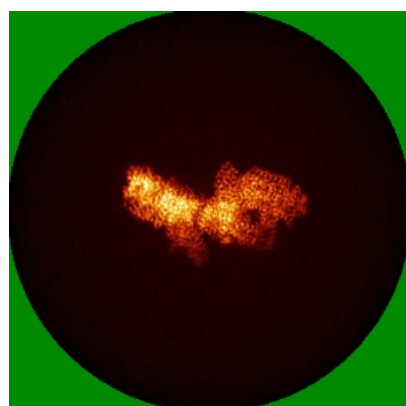


Z Index: 207

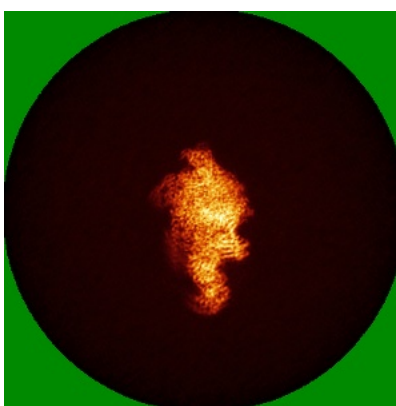
The images above show the largest variance slices of the map in three orthogonal directions.

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

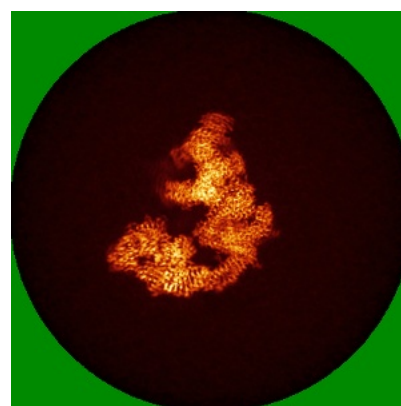
6.4.1 Primary map



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

This section was not generated.

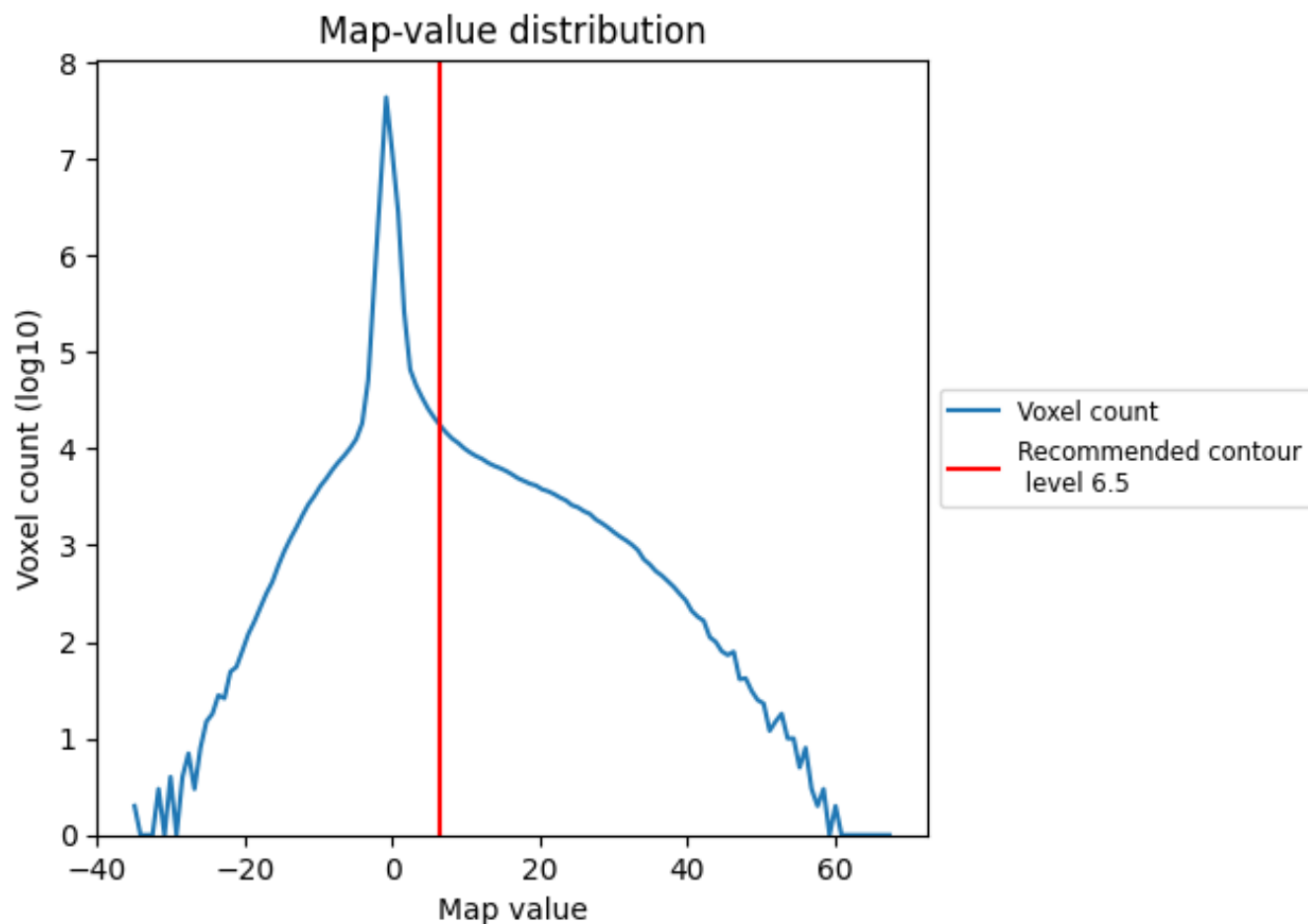
6.6 Mask visualisation

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

7 Map analysis [i](#)

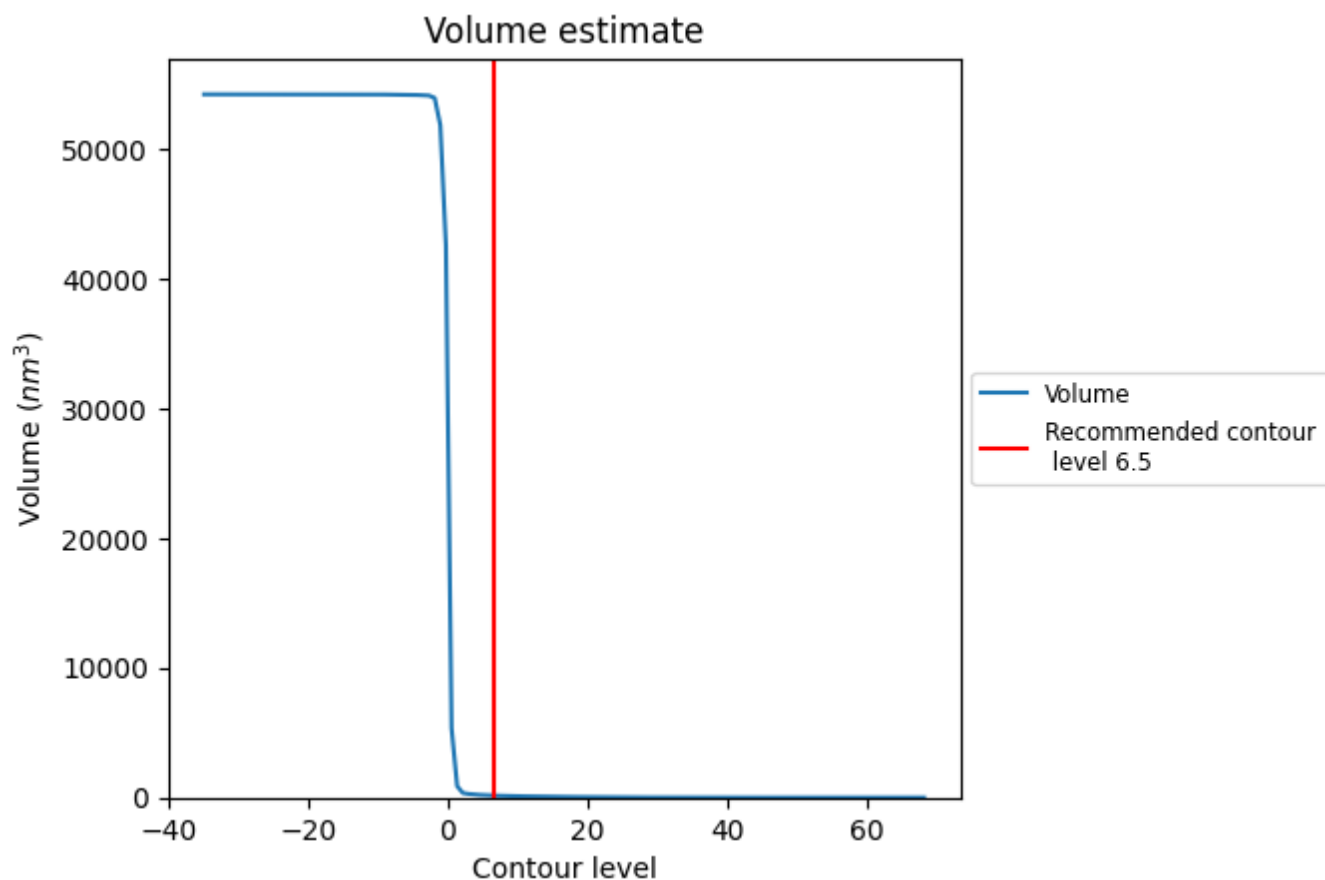
This section contains the results of statistical analysis of the map.

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.

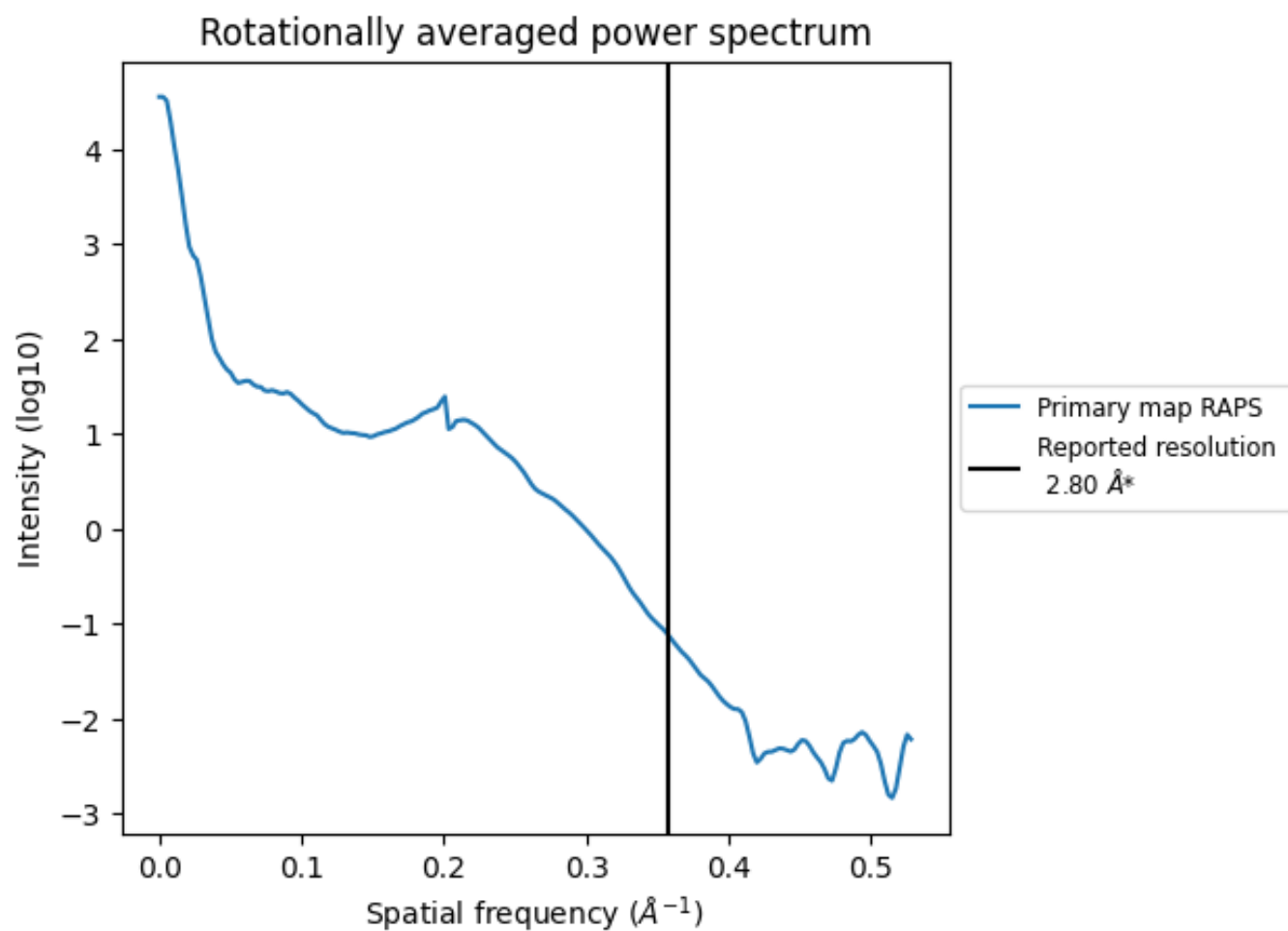
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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.

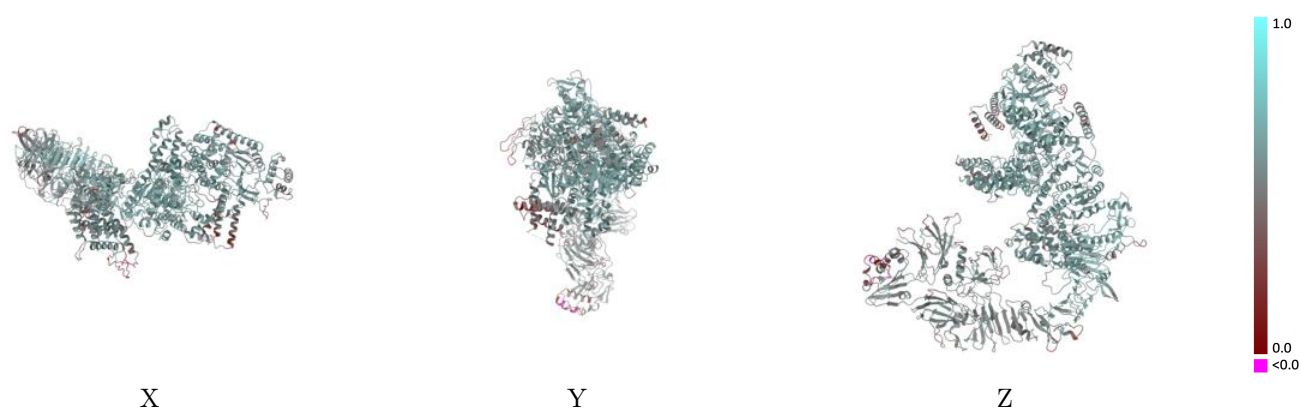
9 Map-model fit [i](#)

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](#)

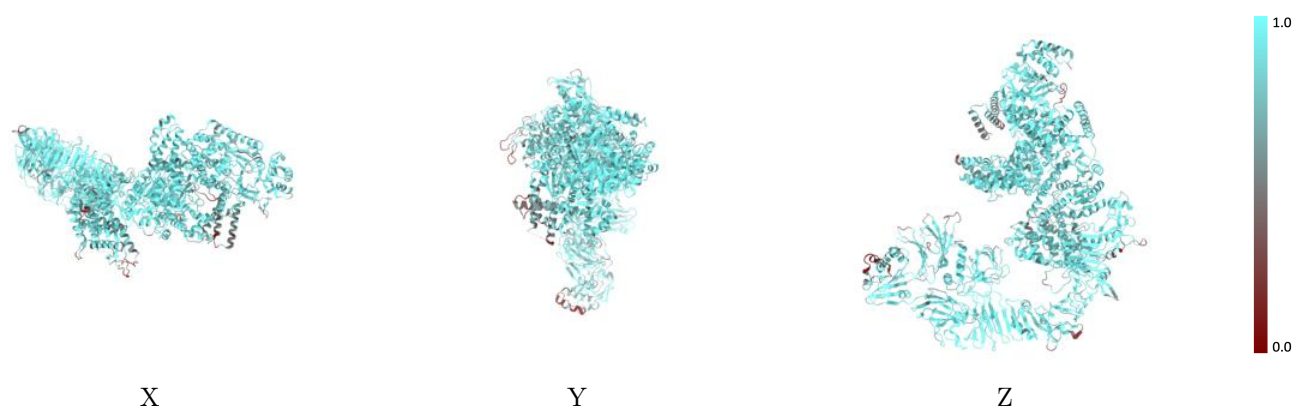
This section was not generated.

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



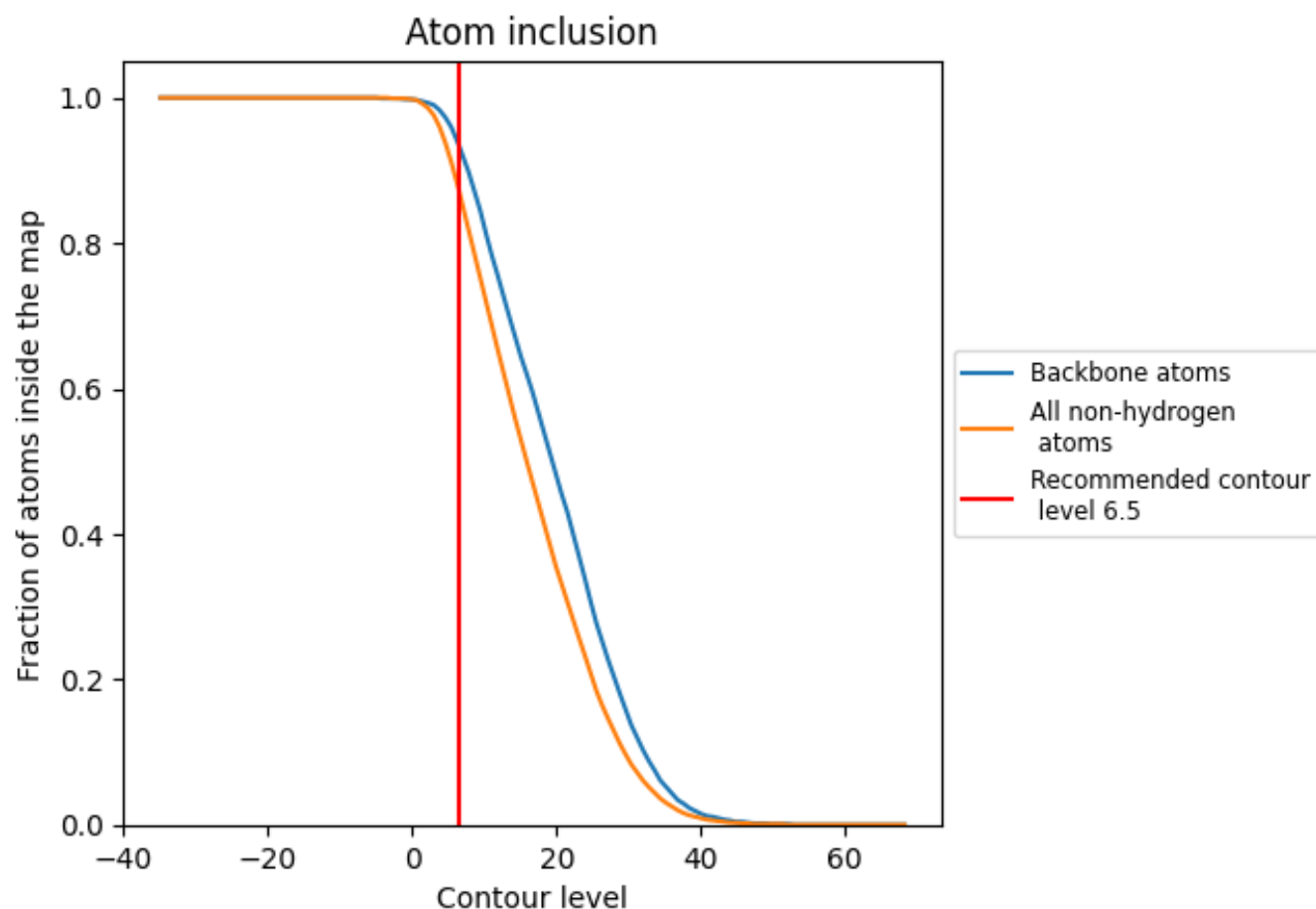
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.4 Atom inclusion ⓘ



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	0.8720	0.5430
A	0.8720	0.5430

