



wwPDB EM Validation Summary Report ⓘ

Jul 9, 2025 – 01:35 am BST

PDB ID : 9QHH / pdb_00009qhh
EMDB ID : EMD-53169
Title : Lymphostatin - pH 8 - phosphate buffer
Authors : Griessmann, M.; Schneider, R.; Rasmussen, T.; Bottcher, B.
Deposited on : 2025-03-15
Resolution : 3.10 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.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

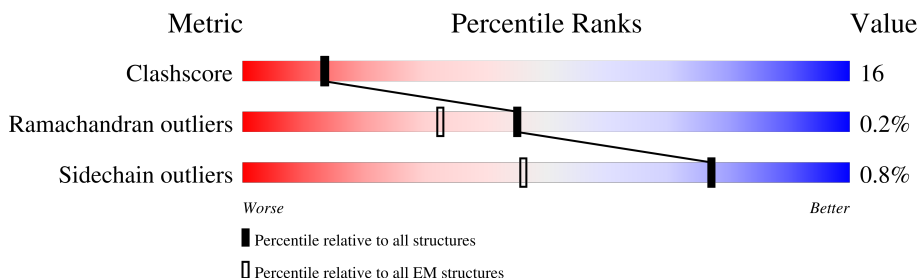
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	

2 Entry composition

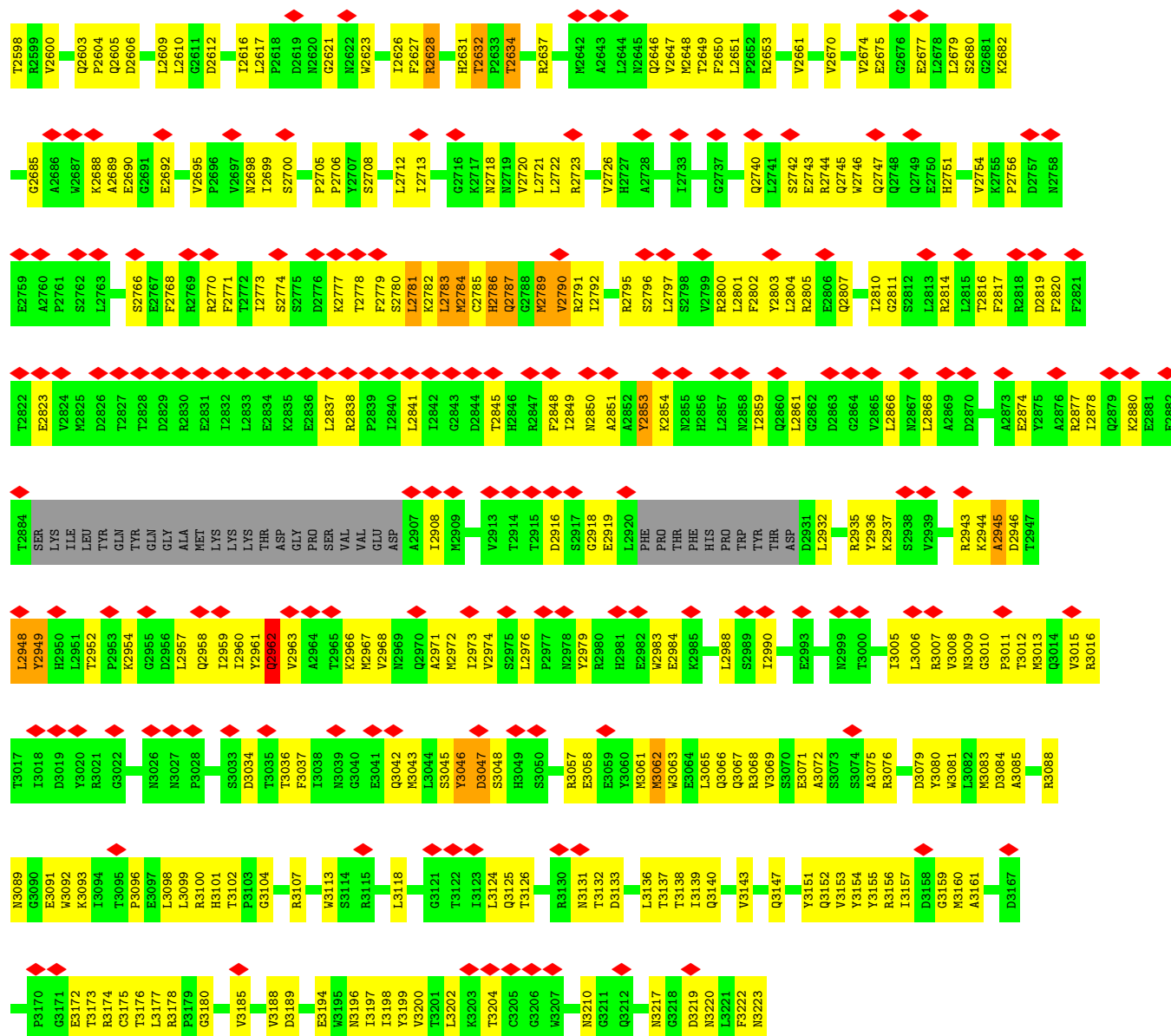
There is only 1 type of molecule in this entry. The entry contains 22339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			22339	14119	3874	4270	76		

T2515	T2516	R2432	R2433	G2303	S2173	G2020	LEU	R1802	L1665	P1519	L1373	P1237	ASP	E488
T2517	A2517	E2433	N2434	G2309	N2174	S2030	ALA	G1805	Q1666	P1520	L1377	P1248	PHE	E489
T2518	T2518	G2435	N2435	G2312	I2176	S2031	LYS	R1806	L1667	L1520	L1378	P1259	LEU	K853
G2520	T2519	G2436	L2436	T2312	D2184	S2032	ASN	H1807	T1668	D1524	G1379	E1251	GLU	Q862
T2521	G2314	G2315	G2315	R2034	S2187	A2033	LEU	L1808	D1671	M1528	P1378	L1252	ARG	A863
T2527	G2325	G2439	G2439	R2034	R2188	R2035	ALA	V1810	A1674	M1529	K1382	L1253	LYS	S864
T2528	T2326	N2440	N2440	R2035	H2189	V2036	M1897	E1811	V1682	Q1539	L1383	P1255	ILE	T867
N2529	G2327	S2441	S2441	A2037	K2190	A2037	K1899	N1812	K1690	N1548	R1386	P1256	ASN	K868
K2530	D2327	R2447	R2447	R2038	R2191	R2038	Q1901	T1813	K1690	E1549	E1387	L1257	MET	K869
P2531	D2328						L1902	E1814	L1690	S1550	Q1399	V1257	SER	D870
T2534	D2329						S1903	L1815	T1698	L1551	Q1399	V1261	LYS	L871
T2537	N2330	Y2451	Y2451	G2331	Q2200	H2043	E1904	F1823	L1699	T1555	F1414	S1269	ASP	K874
P2538	F2332	E2455	E2455	F2332	T2202	Q2045	T1906	L1824	D1700	N1558	N1415	E1277	THR	K874
T2541	N2341	N2456	N2456	V2341	E2207	F2052	M1910	Q1826	R1702	Q1559	I1418	Q1278	GLU	S889
T2542	T2342	D2460	D2460	T2342	L2215	T2060	I1911	R1827	I1704	I1562	I1419	V1279	LEU	D892
L2543	N2347	A2461	A2461	N2347	R2216	A2063	F1918	D1828	L1732	R1573	E1433	V1280	TRP	F993
A2544	P2353	L2462	L2462	P2353	D2220	L2069	L1919	D1829	T1733	H1581	H1434	V1281	GLU	K894
T2553	L2360	R2463	R2463	L2360	Q2228	L2070	R1928	H1834	E1735	L1594	E1445	G1282	LYS	N895
L2556	H2371	M2469	M2469	H2371	S2231	F2078	E1930	T1836	Q1736	T1595	F1445	V1283	ARG	M802
P2560	L2375	L2473	L2473	L2375	L2239	K2080	S1931	V1838	D1738	D1596	Y1446	G1283	VAL	M905
T2561	T2378	T2474	T2474	T2378	L2239	M2081	A1932	V1840	I1740	N1598	R1447	H1305	GLN	I906
L2562	T2379	V2477	V2477	T2379	S2243	D2109	M1937	F1847	R1741	H1601	S1462	H1306	LEU	M907
V2563	L2380	R2478	R2478	L2380	V2250	G2111	V1940	Q1848	I1743	D1603	E1446	V1307	TYR	L908
K2566	V2386	F2479	F2479	V2386	G2251	D2112	M1948	K1849	Q1747	F1604	I1465	R1308	LEU	D913
T2567	T2484	T2484	T2484	T2484	G2252	V2113	T1947	L1850	I1747	L1605	D1466	M1309	TRP	I914
D2568	Y2488	Y2488	Y2488	Y2488	I2258	Q2114	G1949	M1853	R1750	S1606	Q1470	H1310	GLU	E928
V2572	D2489	P2490	P2490	D2489	N2267	T2115	L1959	L1857	R1754	D1609	L1472	L1314	LEU	N839
T2574	T2574	N2399	N2399	T2574	T2268	R2116	L1959	L1857	R1754	A1610	L1472	N1315	GLN	Y944
L2576	Q2493	Q2493	Q2493	Q2493	L2269	V2119	I1978	M1869	T1764	F1613	T1476	Q1317	LEU	L947
T2577	L2495	L2495	L2495	L2495	S2270	A2122	Q1979	S1870	Q1765	T1614	Q1476	N1318	SER	H948
Q2580	V2496	V2496	V2496	V2496	F2271	R2122	L1980	V1872	D1766	E1615	E1477	L1319	LYS	K949
L2583	Q2498	Q2498	Q2498	Q2498	R2272	N2137	Y1986	G1873	L1768	E1626	M1481	L1323	GLN	N966
Q2584	H2412	H2412	H2412	H2412	L2280	K2146	S1987	V1874	V1769	L1631	L1488	S1329	ALA	K970
L2585	F2413	F2413	F2413	F2413	T2281	T2147	E1988	V1875	S1770	L1631	Q1489	L1341	ASN	L974
T2586	A2414	A2414	A2414	A2414	F2282	L2147	A1991	Q1876	Q1772	V1641	T1490	S1342	PHE	Y975
L2587	G2415	G2415	G2415	G2415	D2283	Y2159	S2002	R1879	K1783	W1650	E1491	E1345	LEU	S976
S2588	D2423	D2423	D2423	D2423	S2285	V2166	T2006	Q1883	Q1784	N1650	Y1496	H1356	ILE	E980
G2589	G2424	G2424	G2424	G2424	V2291	T2167	T2006	G1884	L1793	N1651	N1502	H1356	THR	H981
L2590	N2425	N2425	N2425	N2425	K2294	E2168	S2009	H1885	F1797	L1653	L1503	A1366	GLU	N982
P2595	T2426	T2426	T2426	T2426	K2294	E2170	L2015	ASP	F1797	L1654	V1506	D1367	LYS	I983
E2596	L2427	L2427	L2427	L2427	D2298	L2172	I2016	SER	I1800	T1663	L1509	A1368	THR	F984
T2597	A2429	A2429	A2429	A2429				THR	P1801	R1664		T1369	GLU	I985
													ASN	K986



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1294835	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)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	38.760	Depositor
Minimum map value	-16.272	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.866	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](#)

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	0.29	0/22776	0.48	7/30862 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2945	ALA	N-CA-C	-11.01	99.66	112.87
1	A	2787	GLN	N-CA-C	-8.61	101.81	111.71
1	A	2781	LEU	N-CA-C	-6.57	104.12	111.28
1	A	1524	ASP	N-CA-C	-6.00	106.94	114.56
1	A	1419	ILE	N-CA-C	-5.65	107.78	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	22339	0	22342	704	0
All	All	22339	0	22342	704	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 16.

The worst 5 of 704 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:2774:SER:HB3	1:A:2780:SER:HB2	1.25	1.15
1:A:2773:ILE:HD11	1:A:2783:LEU:HG	1.35	1.04
1:A:2961:TYR:HB2	1:A:2972:MET:HE3	1.47	0.95
1:A:2944:LYS:H	1:A:2962:GLN:HE22	1.08	0.94
1:A:2962:GLN:HA	1:A:2971:ALA:HA	1.51	0.92

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%)	2684 (96%)	102 (4%)	5 (0%)	44 74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2634	THR
1	A	2790	VAL
1	A	2962	GLN
1	A	3047	ASP
1	A	2963	VAL

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	2491/2880 (86%)	2470 (99%)	21 (1%)	79 89

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2853	TYR
1	A	2959	ILE
1	A	3062	MET
1	A	2962	GLN
1	A	2949	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1250	HIS
1	A	3140	GLN
1	A	1502	ASN
1	A	2758	ASN
1	A	1417	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 ⓘ

There are no chain breaks in this entry.

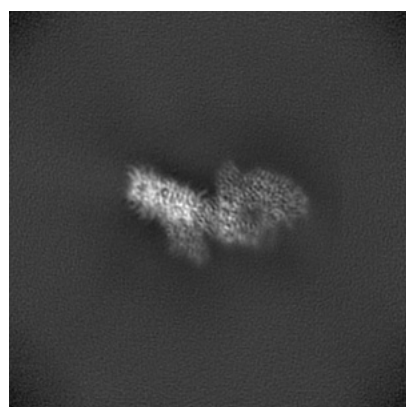
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53169. These allow visual inspection of the internal detail of the map and identification of artifacts.

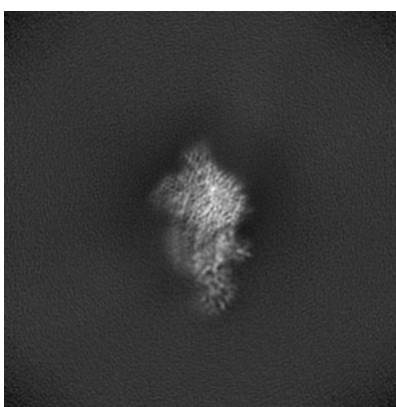
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

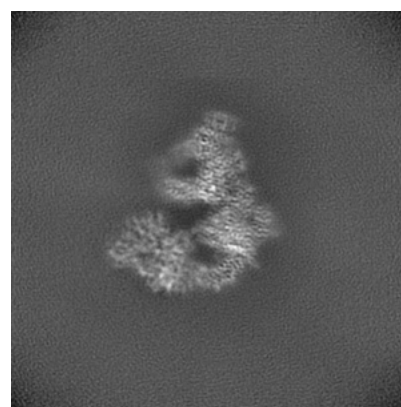
6.1.1 Primary map



X



Y

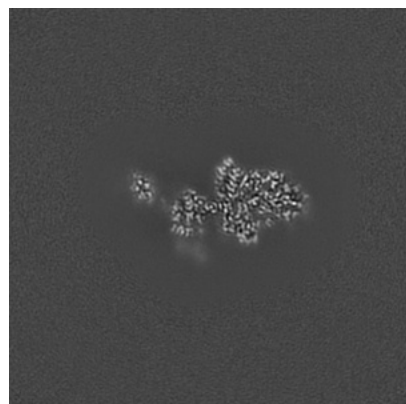


Z

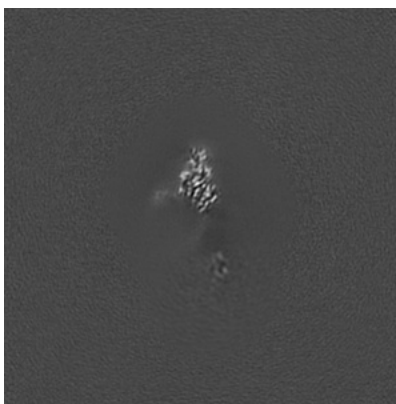
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

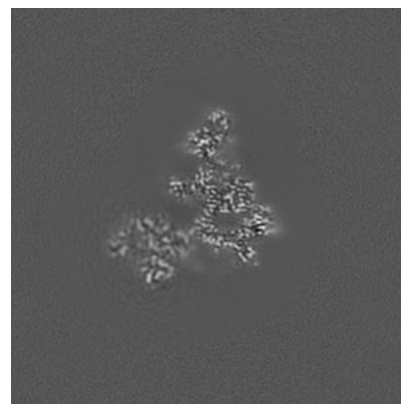
6.2.1 Primary map



X Index: 200



Y Index: 200

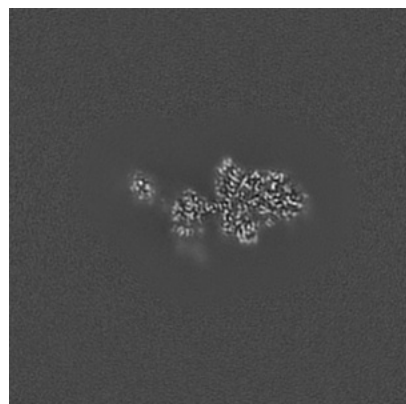


Z Index: 200

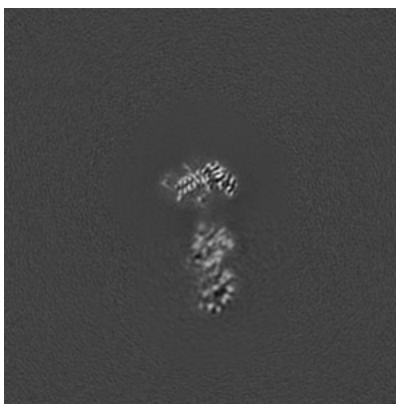
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

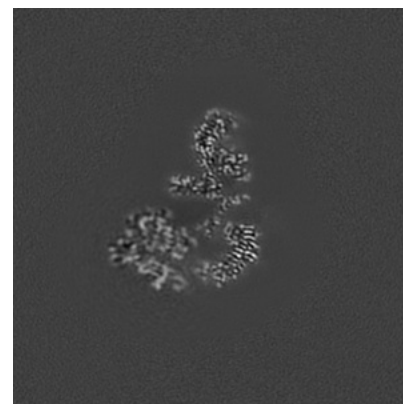
6.3.1 Primary map



X Index: 199



Y Index: 160

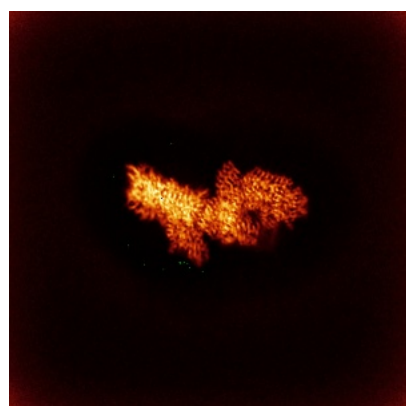


Z Index: 212

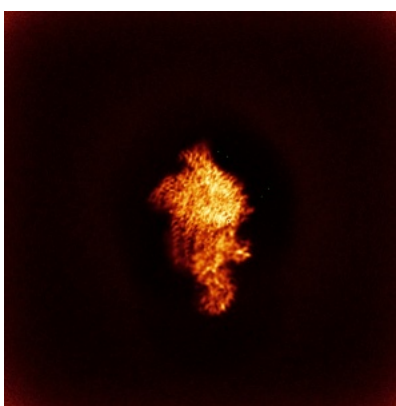
The images above show the largest variance slices of the map in three orthogonal directions.

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

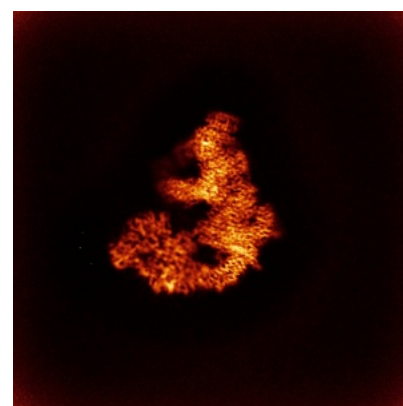
6.4.1 Primary map



X



Y

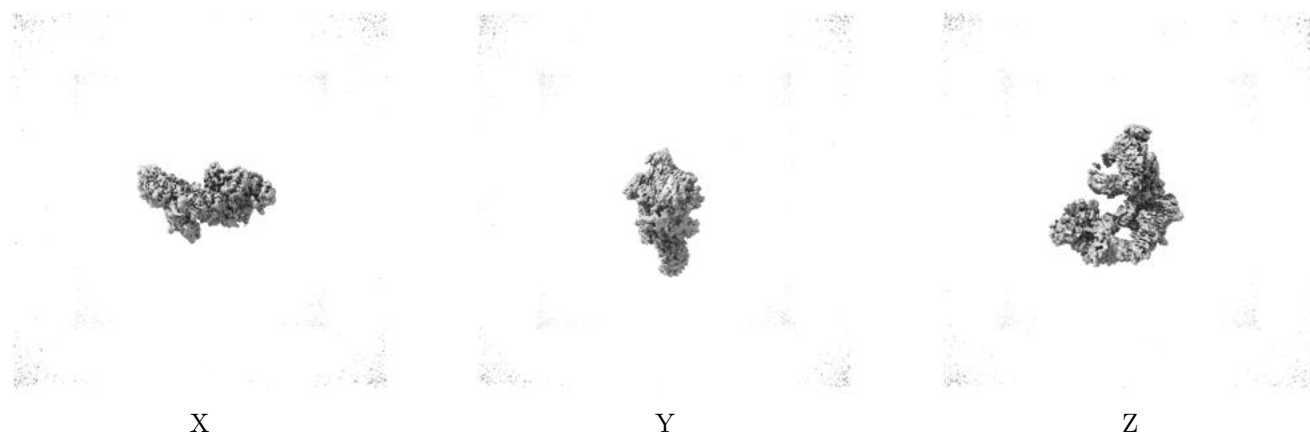


Z

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.

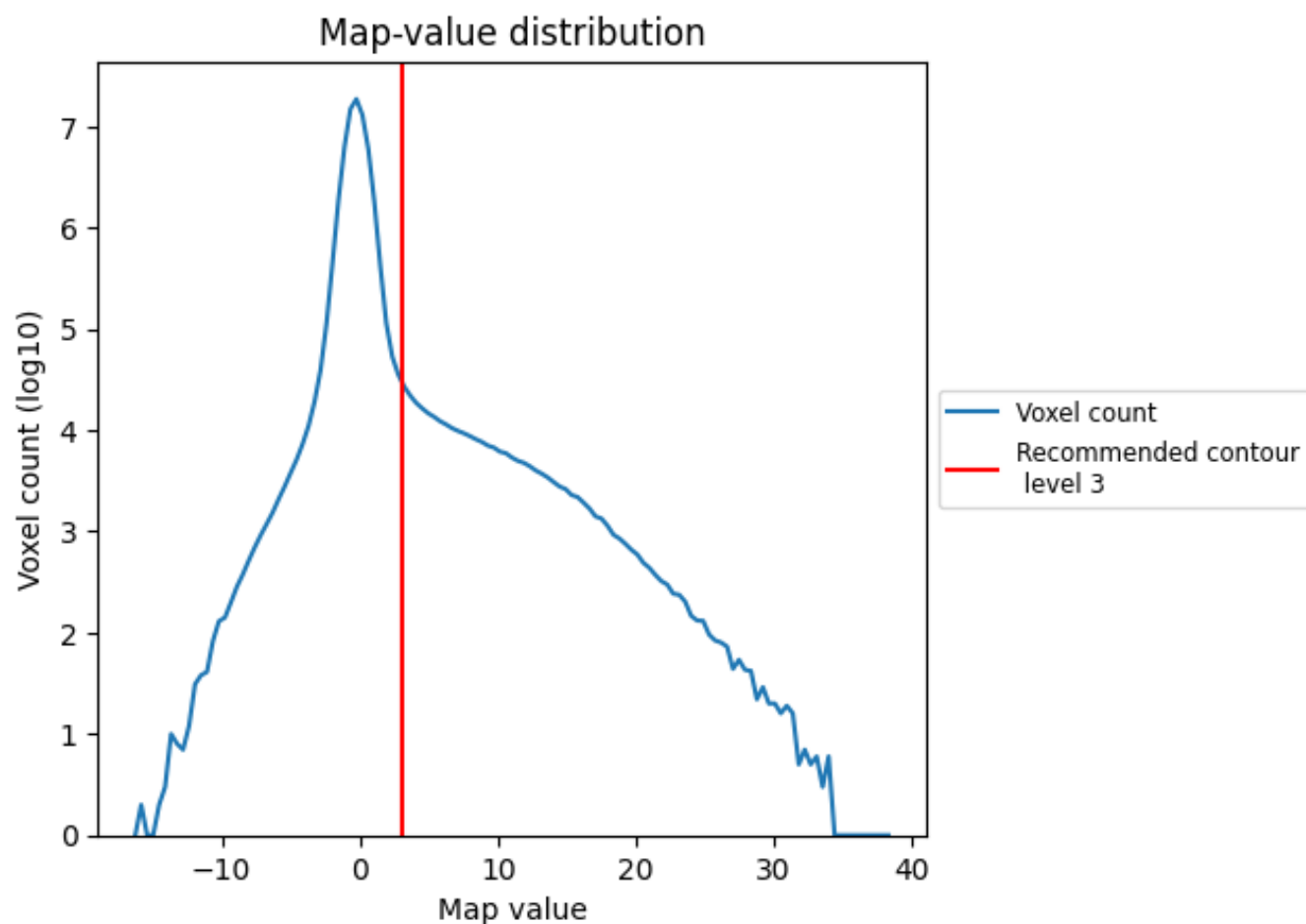
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

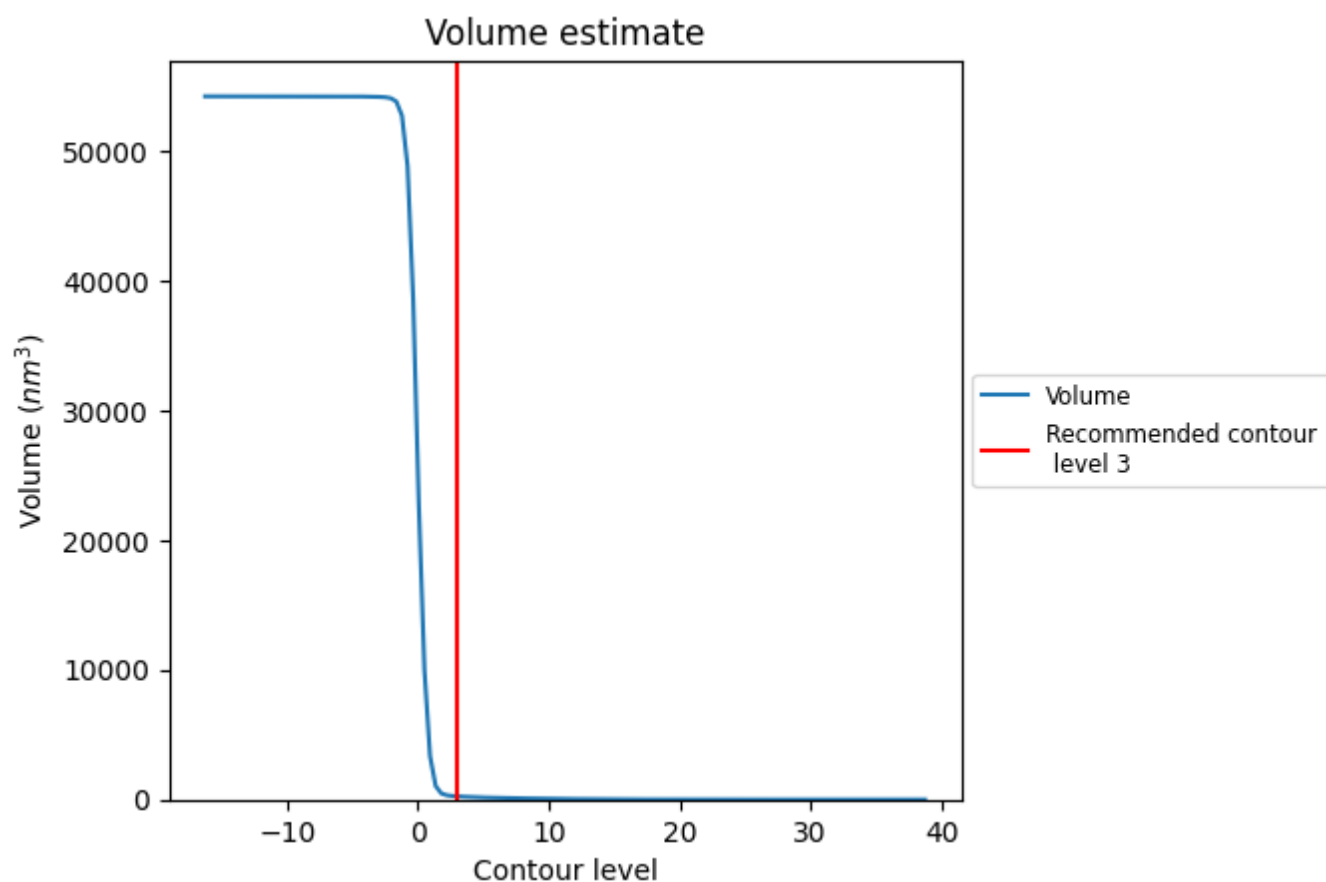
This section contains the results of statistical analysis of the map.

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.

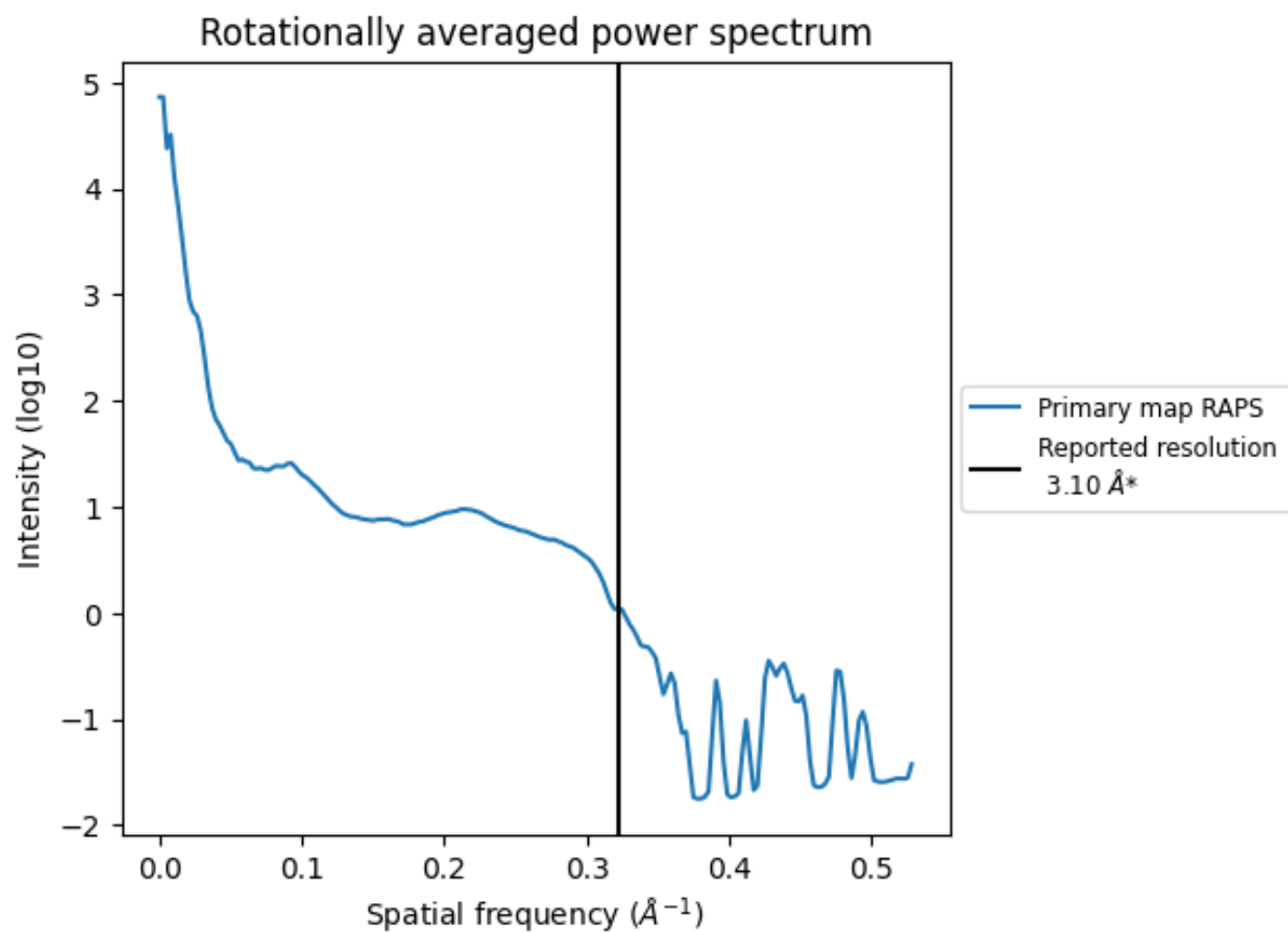
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 248 nm^3 ; this corresponds to an approximate mass of 224 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 0.323 Å⁻¹

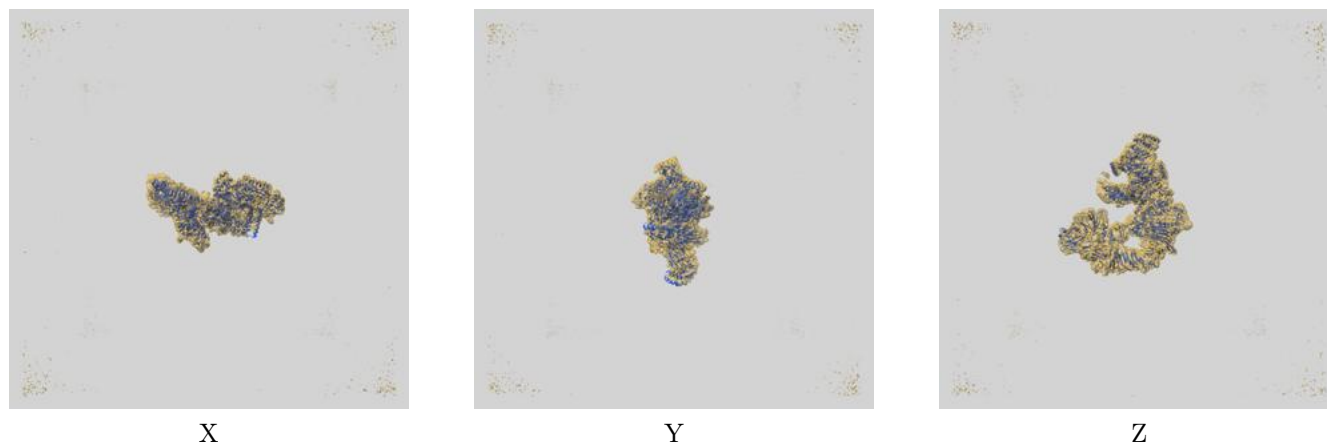
8 Fourier-Shell correlation

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-53169 and PDB model 9QHH. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



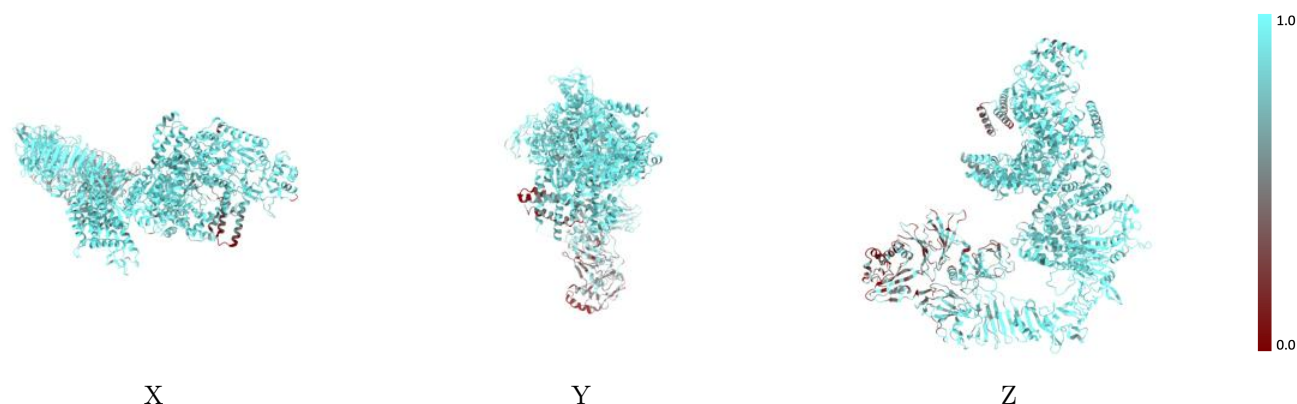
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



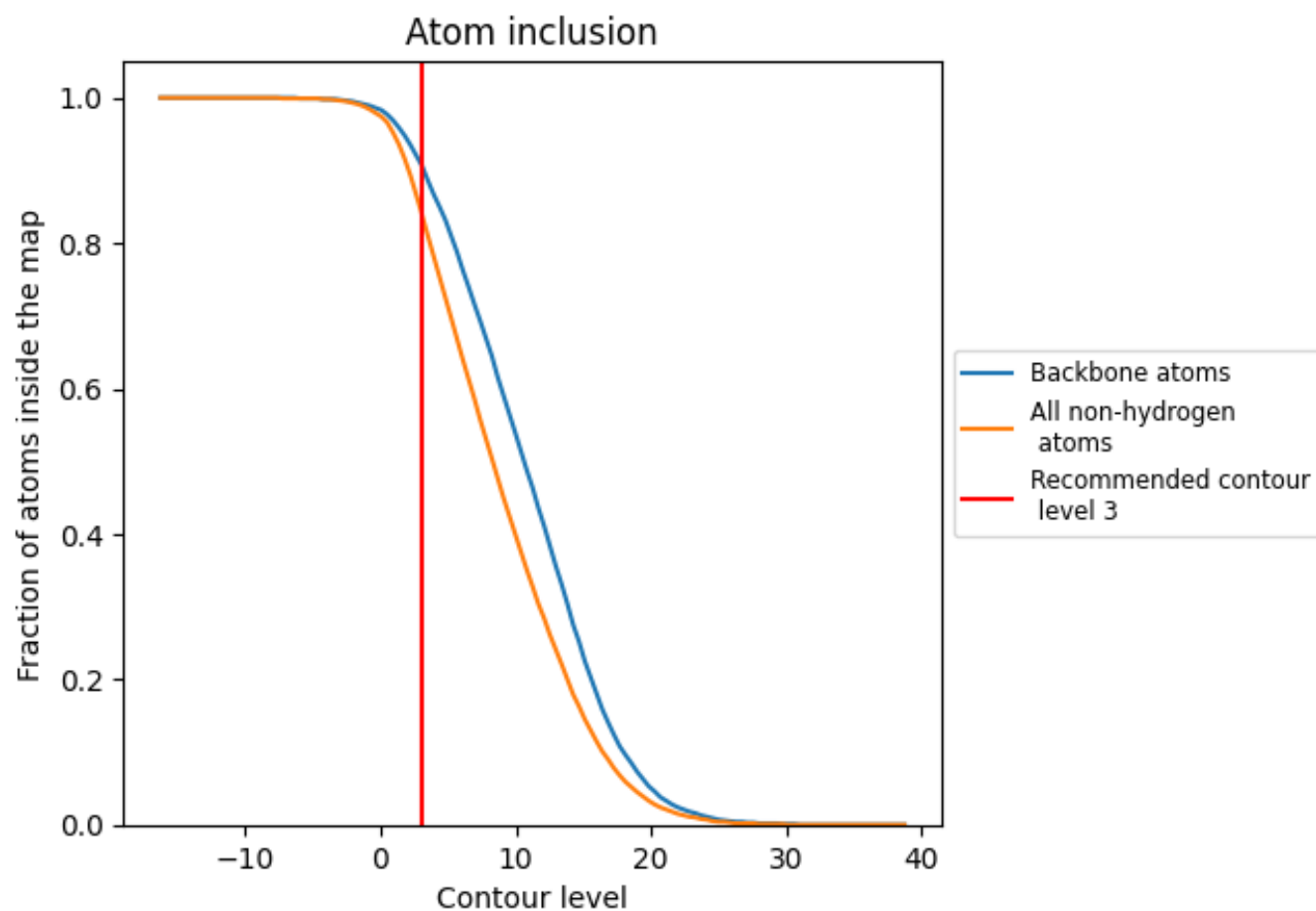
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% of all backbone atoms, 84% 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></div></div> 0.8440	<div><div></div></div> 0.3800
A	<div><div></div></div> 0.8440	<div><div></div></div> 0.3800

