



wwPDB EM Validation Summary Report ⓘ

Apr 28, 2026 – 12:22 PM JST

PDB ID : 9XE7 / pdb_00009xe7
EMDB ID : EMD-66784
Title : Crimean-Congo hemorrhagic fever virus RNA polymerase containing a 10-bp RNA product and incorporated cytidine
Authors : Xue, L.; Gui, J.; Pan, H.; Chang, T.; Xiong, X.
Deposited on : 2025-10-27
Resolution : 3.02 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

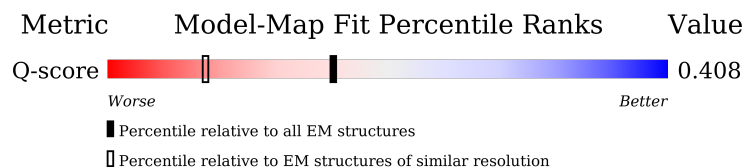
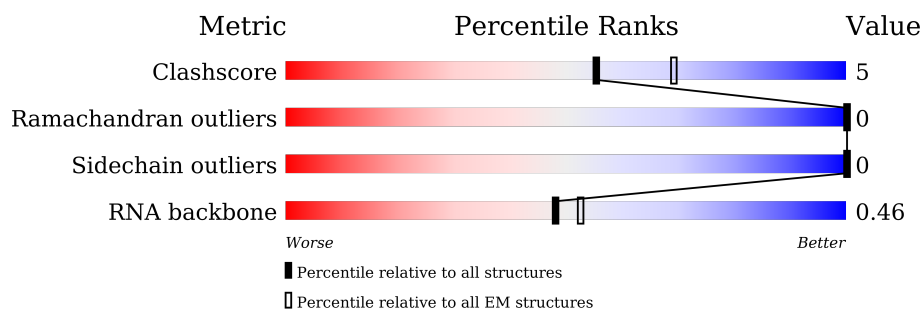
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.02 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	13913 (2.52 - 3.52)

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	3945	
2	B	19	
3	C	19	

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Mol	Chain	Length	Quality of chain
3	E	19	 21% 16% 5% 58%
4	D	10	 40% 50% 10%
5	F	4	 50% 50%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26422 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3182	Total	C	N	O	S	0	0
			25457	16170	4353	4770	164		

- Molecule 2 is a RNA chain called RNA (5'-R(*UP*UP*CP*CP*AP*AP*AP*AP*AP*AP*UP*CP*GP*UP*UP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	11	Total	C	N	O	P	0	0
			231	106	45	70	10		

- Molecule 3 is a RNA chain called RNA (5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*GP*UP*CP*UP*UP*UP*GP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	12	Total	C	N	O	P	0	0
			258	115	46	85	12		
3	E	8	Total	C	N	O	P	0	0
			170	76	29	57	8		

- Molecule 4 is a RNA chain called RNA (5'-R(*UP*CP*UP*CP*AP*AP*AP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	9	Total	C	N	O	P	0	0
			191	86	36	60	9		

- Molecule 5 is a RNA chain called RNA (5'-R(P*UP*CP*UP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	4	Total	C	N	O	P	0	0
			81	36	10	31	4		

- Molecule 6 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]amino}phosph

The chemical structure of 2KH is a complex molecule. It features a pyridine ring (blue) at the bottom, which is connected to a ribose sugar (brown) via a nitrogen atom (N1). The ribose sugar is further connected to a phosphate chain (purple) via an oxygen atom (O1). The phosphate chain consists of three phosphate groups (P1, P2, P3) linked by oxygen atoms (O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799, O800, O801, O802, O803, O804, O805, O806, O807, O808, O809, O810, O811, O812, O813, O814, O815, O816, O81

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

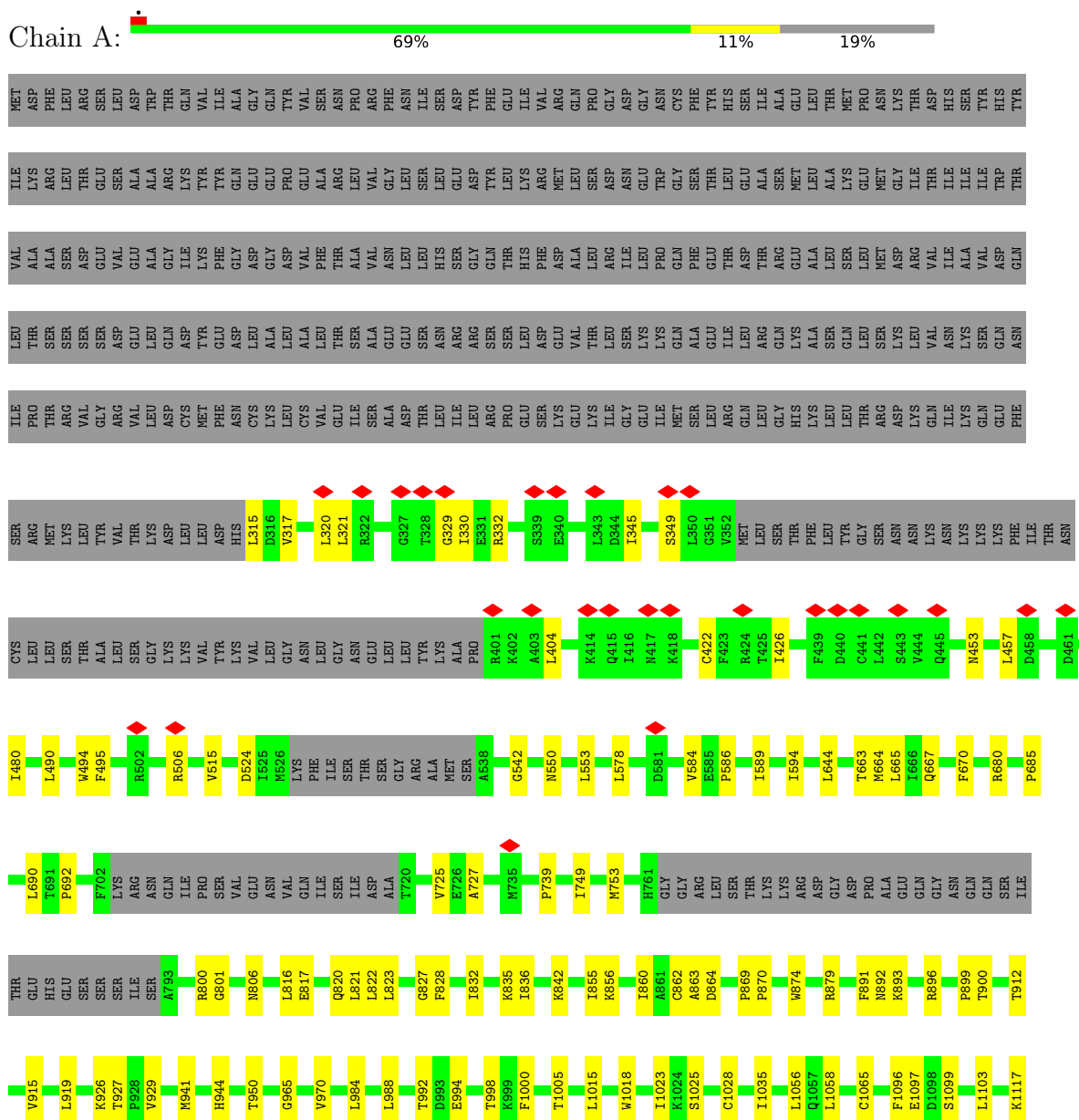
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

WORLDWIDE
 **PDB**
PROTEIN DATA BANK

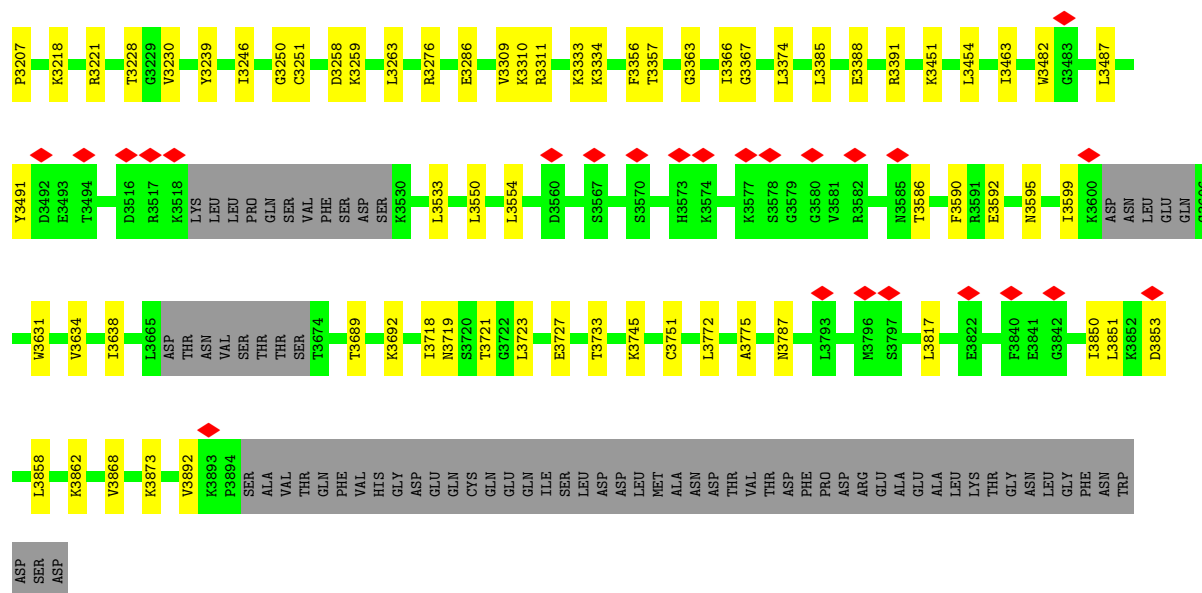
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA-directed RNA polymerase L

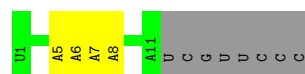


H3045	L2867	ALA	Y2622	C2398	K2216	GLU	R1943	E1843	ARG	V1596	I1363	H1184
V3048	I2868	SER	V2528	V2401	E2217	LEU	L1944	I1847	SER	I1611	K1373	GLY
F3053	P2869	HIS	L2218	P2404	L2219	ILE	K1945	L1950	TYR	H1615	L1383	VAL
L3068	L2872	ASP	L2636	L2419	T2219	ASN	H1950	G1953	SER	H1621	L1386	SER
E2875	L2872	GLY	L2640	L2419	ARG	SER	PRU	LYS	LYS	G1627	L1395	ALA
Q3066	E2875	SER	L2655	R2434	THR	GLU	GLU	LYS	ARG	Q1396	L1419	HIS
R3069	L2876	SER	T2856	R2435	GLU	LEU	LEU	LYS	ILE	P1397	Y1411	ASN
I3070	L2867	SER	L2657	L2436	GLU	PRU	GLU	GLY	ARG	R1638	Q1424	ASP
A3082	L2660	SER	L2660	S2459	ARG	L2141	ASN	ALA	SER	I1657	L1499	GLY
V3088	E2744	ASP	V2148	L2227	L2227	V2148	ASN	ILE	ILE	L1663	Y1502	ASN
K3089	E2756	GLY	L2232	H2477	R2232	M2068	C1959	SER	PHE	P1668	V1502	LEU
V3099	L2760	SER	L2670	L2486	L2251	E2069	L1960	THR	GLY	Y1503	Y1503	LYS
L3100	K2761	SER	L2674	A2487	Q2252	T2070	E1964	ILE	TYR	F1505	I1414	ASP
L3101	L2763	ASP	A2268	Y2498	A2268	F2075	E1965	GLU	ASN	L1418	T1417	SER
P3105	Q2776	GLY	V2269	V2510	L2270	F2076	N1967	ILE	TYR	Y1419	Q1424	ASP
K3109	L2779	LEU	A2271	S2515	P2272	L2079	I1970	G1868	GLN	Q1499	L1657	GLN
G3110	L2797	ASP	K2273	S2516	K2273	K2088	K1973	R1870	PHE	L1663	L1663	ARG
Y3111	L2881	ASP	R2280	D2517	L2270	ALA	K1974	I1894	GLU	L1663	L1663	LEU
L3112	L2887	LEU	D2281	L2523	L2270	LEU	L1975	I1894	LEU	P1668	V1502	LEU
K2954	L2694	LEU	L2282	Y2537	L2282	GLY	L1977	P1997	ARG	Y1503	Y1503	ARG
K2959	S2700	THR	T2287	F2541	T2287	THR	ASN	SER	SER	F1505	F1505	ASP
W2970	L2701	THR	V2291	R2547	V2291	THR	GLN	LYS	LYS	L1506	L1506	ASP
W2970	S2705	LEU	T2295	T2552	T2295	LEU	GLN	PHE	ALA	L1507	L1507	ALA
D3134	L2830	THR	K2305	V2555	V2555	VAL	GLN	GLU	ALA	K1508	K1508	ALA
R3135	A2833	LEU	G2311	M2561	M2561	ASP	GLN	GLU	ASN	L1512	L1512	ASN
F3136	G2840	ASP	L2312	L2569	L2312	GLY	GLN	GLU	GLY	R1526	R1526	GLY
L3137	GLY	THR	L2335	S2570	L2335	THR	LEU	LEU	LYS	G1532	G1532	LYS
M3139	GLY	LEU	L2348	L2574	L2348	THR	LYS	L1908	LEU	L1533	L1533	LEU
Q3140	GLY	GLY	C2354	M2582	C2354	GLY	LYS	V1909	LEU	S1534	S1534	LEU
F3141	THR	THR	M2359	A2589	M2359	ILE	GLY	K1910	LEU	R1535	R1535	LYS
L3152	GLY	GLY	K2361	V2590	K2361	THR	I1996	K1911	LEU	L1536	L1536	LEU
R3173	VAL	VAL	W2362	T2591	W2362	GLY	I1998	R1912	ASN	V1537	V1537	ASN
L3178	ALA	ALA	M2374	F2593	M2374	ASP	S1993	I1913	ASP	C1538	C1538	SER
L3181	LEU	LEU	D2384	F2595	D2384	THR	S1994	I1916	THR	P1539	P1539	ASP
M3184	ASN	ASN	S2387	Q2618	S2387	LEU	I1996	L1917	SER	L1562	L1562	THR
V3194	ASP	ASP	K2395	Q2618	K2395	LEU	I1997	L1918	THR	G1568	G1568	THR
F3195	VAL	VAL	Q2618	Q2618	Q2618	L2114	K1998	E1920	GLN	V1573	V1573	GLN
L3202	SER	SER	Q2618	Q2618	Q2618	L2115	I1999	D1921	ILE	V1577	V1577	ILE
V3041	THR	THR	Q2618	Q2618	Q2618	L2116	D2010	I1932	ALA	W1580	W1580	ALA
						K2120	Q2013	S1933	SER	V1321	V1321	SER
						L2121	K2014	S1934	GLU	V1342	V1342	GLU
						Q2127	F2015	I1822	VAL	V1589	V1589	VAL
						K2128	I2016	G1938	SER	P1592	P1592	SER
						ASP	Y2017	S1939	ASP	V1358	V1358	ASP
							D2025	L1940	ARG	K1359	K1359	ARG
								K1941				
								K1942				



- Molecule 2: RNA (5'-R(*UP*UP*CP*CP*AP*AP*AP*AP*AP*AP*UP*CP*GP*UP*UP*CP*CP*C)-3')

Chain B: 37% 21% 42%



- Molecule 3: RNA (5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*GP*UP*CP*UP*UP*UP*GP*AP*GP*A)-3')

Chain C: 37% 16% 11% 37%



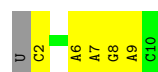
- Molecule 3: RNA (5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*GP*UP*CP*UP*UP*UP*GP*AP*GP*A)-3')

Chain E: 21% 16% 5% 58%



- Molecule 4: RNA (5'-R(*UP*CP*UP*CP*AP*AP*AP*GP*AP*C)-3')

Chain D: 40% 50% 10%



- Molecule 5: RNA (5'-R(P*UP*CP*UP*C)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59907	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.035	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	262.8, 262.8, 262.8	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.876, 0.876, 0.876	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: 2KH, ZN, 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	0.14	0/25891	0.34	0/34920
2	B	0.13	0/259	0.30	0/401
3	C	0.13	0/288	0.22	0/447
3	E	0.16	0/189	0.36	0/292
4	D	0.16	0/213	0.27	0/329
5	F	0.14	0/88	0.40	0/132
All	All	0.14	0/26928	0.34	0/36521

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	25457	0	25876	258	0
2	B	231	0	121	0	0
3	C	258	0	129	4	0
3	E	170	0	86	1	0
4	D	191	0	98	4	0
5	F	81	0	43	2	0
6	A	29	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	4	0	0	0	0
8	A	1	0	0	0	0
All	All	26422	0	26366	264	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 5.

The worst 5 of 264 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:594:ILE:HD11	1:A:893:LYS:HD3	1.72	0.71
1:A:1096:PHE:HB3	1:A:1103:LEU:HD11	1.74	0.70
1:A:1535:ARG:HD3	1:A:1577:VAL:HG11	1.76	0.68
1:A:586:PRO:HD2	1:A:589:ILE:HD13	1.76	0.67
1:A:3388:GLU:HG3	1:A:3391:ARG:HH21	1.59	0.67

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	3138/3945 (80%)	3004 (96%)	134 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	2920/3601 (81%)	2920 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2794	HIS
1	A	3484	HIS
1	A	3497	GLN
1	A	3375	HIS
1	A	2063	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	10/19 (52%)	4 (40%)	0
3	C	11/19 (57%)	2 (18%)	0
3	E	7/19 (36%)	4 (57%)	0
4	D	8/10 (80%)	0	0
5	F	3/4 (75%)	0	0
All	All	39/71 (54%)	10 (25%)	0

5 of 10 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	5	A
2	B	6	A
2	B	7	A
2	B	8	A
3	C	8	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	2KH	A	4001	7	29,30,30	3.95	20 (68%)	42,47,47	1.60	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	2KH	A	4001	7	-	6/19/38/38	0/2/2/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4001	2KH	C3'-C2'	-8.84	1.29	1.53
6	A	4001	2KH	C2-N3	7.03	1.50	1.38
6	A	4001	2KH	C2-N1	6.57	1.49	1.38
6	A	4001	2KH	C6-C5	6.09	1.49	1.35
6	A	4001	2KH	PB-O3B	5.99	1.66	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4001	2KH	C4-N3-C2	-5.02	119.95	126.58
6	A	4001	2KH	N3-C2-N1	4.05	120.27	114.89
6	A	4001	2KH	C5-C4-N3	3.46	120.01	114.84
6	A	4001	2KH	PB-O3B-PG	-2.95	122.24	132.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4001	2KH	O4-C4-C5	-2.78	120.26	125.16

There are no chirality outliers.

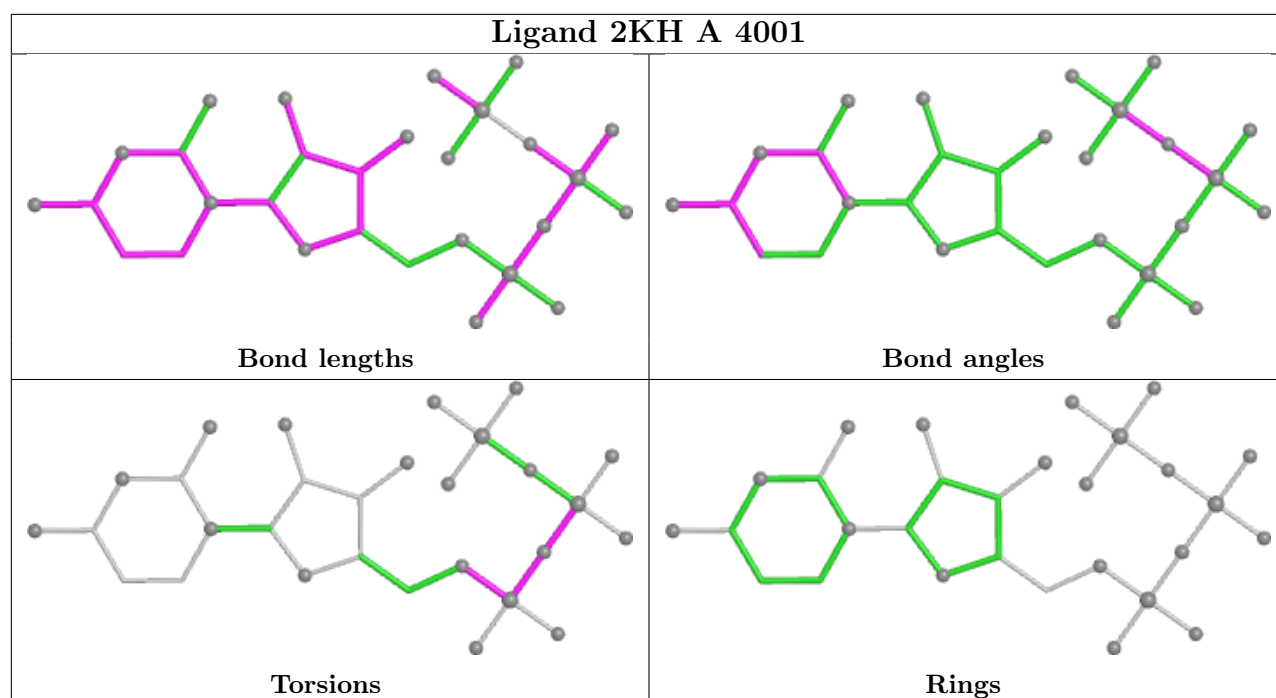
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	4001	2KH	PB-N3A-PA-O1A
6	A	4001	2KH	PB-N3A-PA-O5'
6	A	4001	2KH	C5'-O5'-PA-O2A
6	A	4001	2KH	PA-N3A-PB-O2B
6	A	4001	2KH	PA-N3A-PB-O3B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

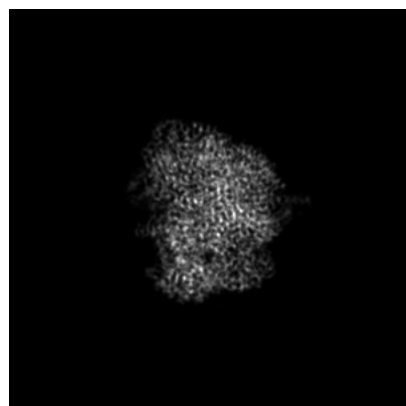
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66784. These allow visual inspection of the internal detail of the map and identification of artifacts.

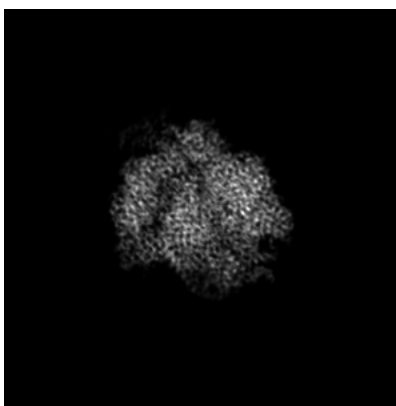
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

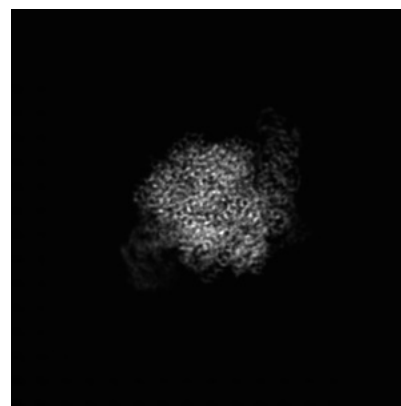
6.1.1 Primary map



X

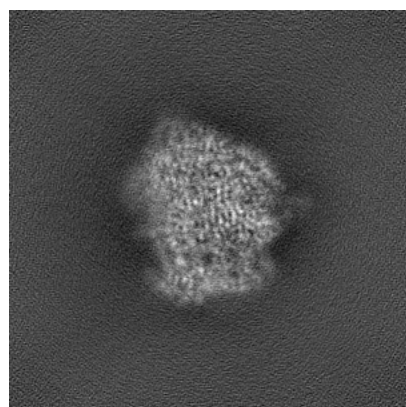


Y

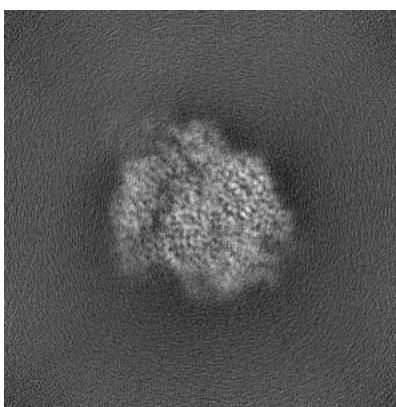


Z

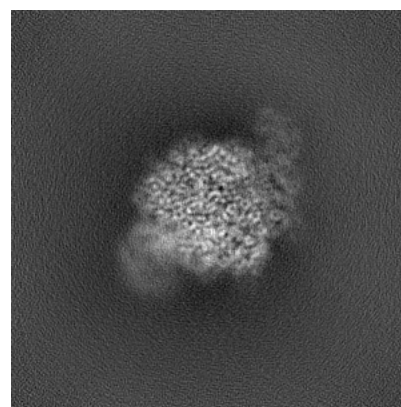
6.1.2 Raw map



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: 150

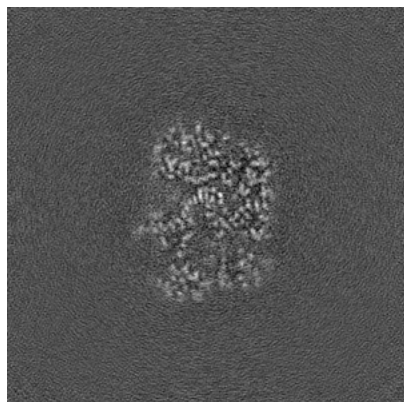


Y Index: 150

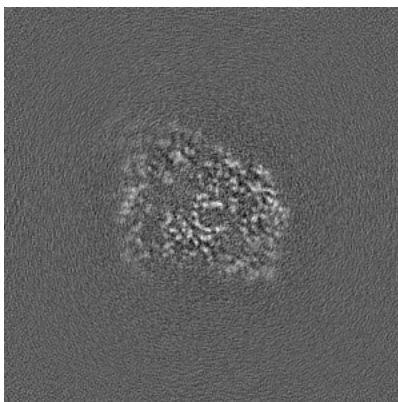


Z Index: 150

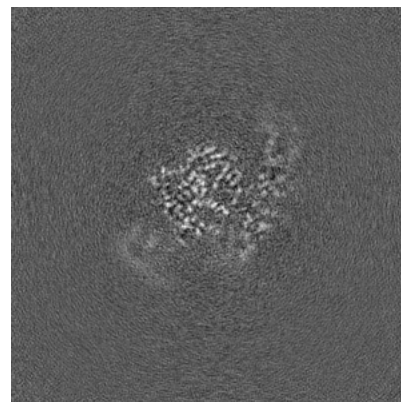
6.2.2 Raw map



X Index: 150



Y Index: 150

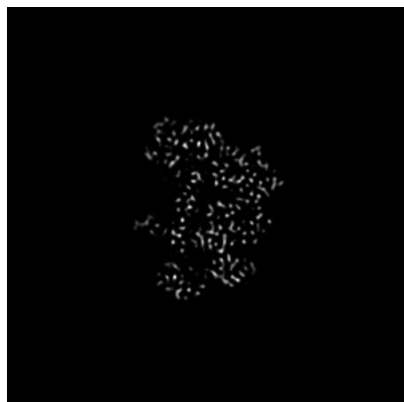


Z Index: 150

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: 143

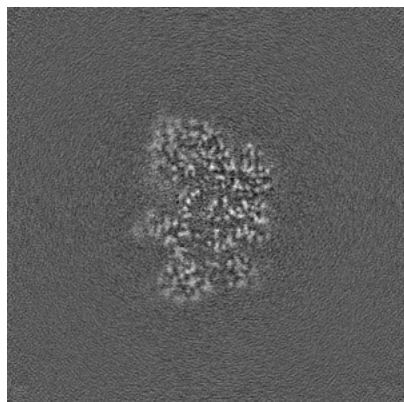


Y Index: 144

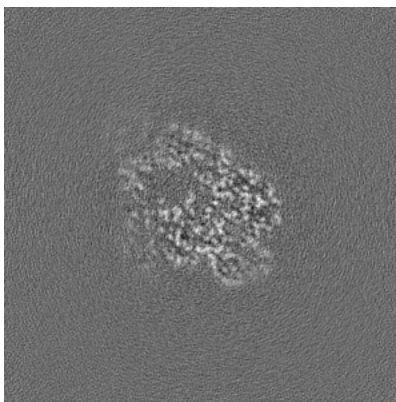


Z Index: 135

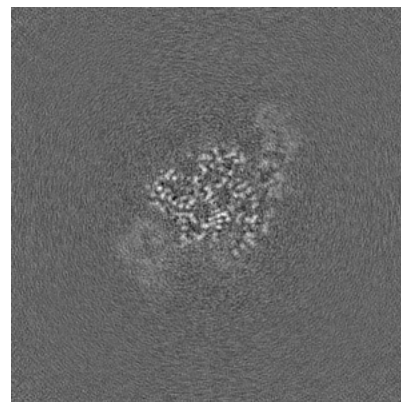
6.3.2 Raw map



X Index: 146



Y Index: 157

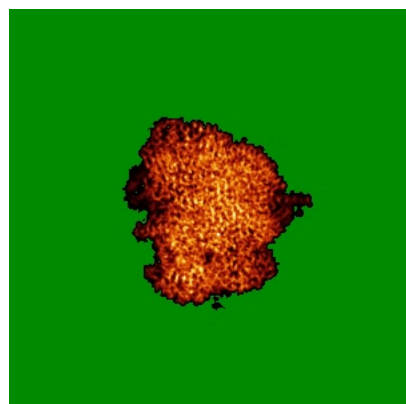


Z Index: 154

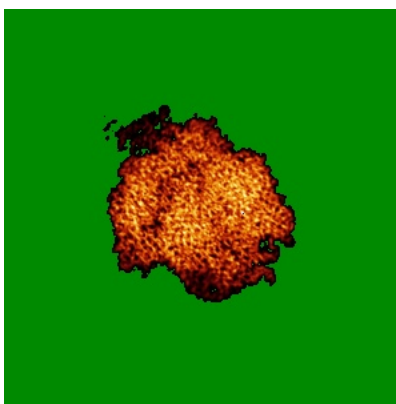
The images above show the largest variance slices of the map in three orthogonal directions.

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

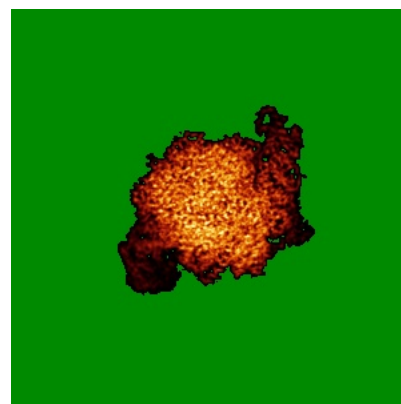
6.4.1 Primary map



X

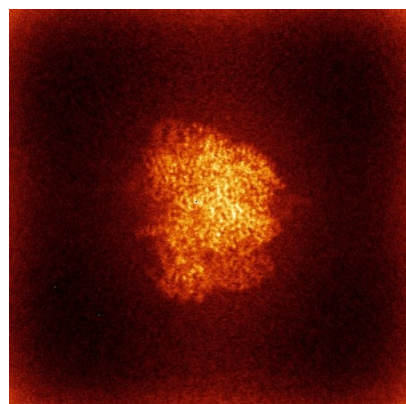


Y

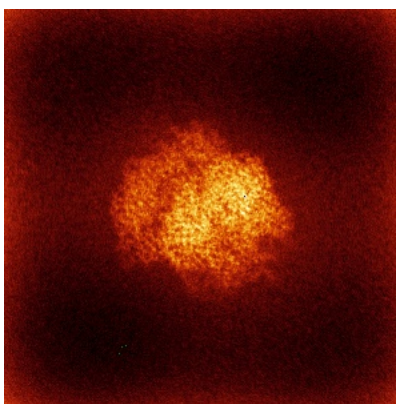


Z

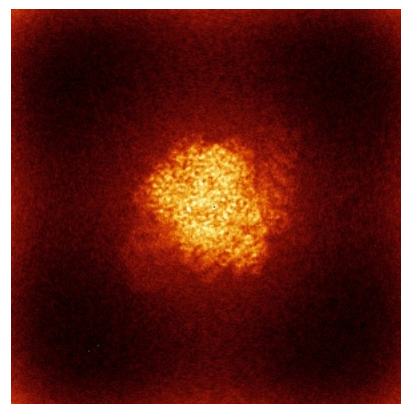
6.4.2 Raw map



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.

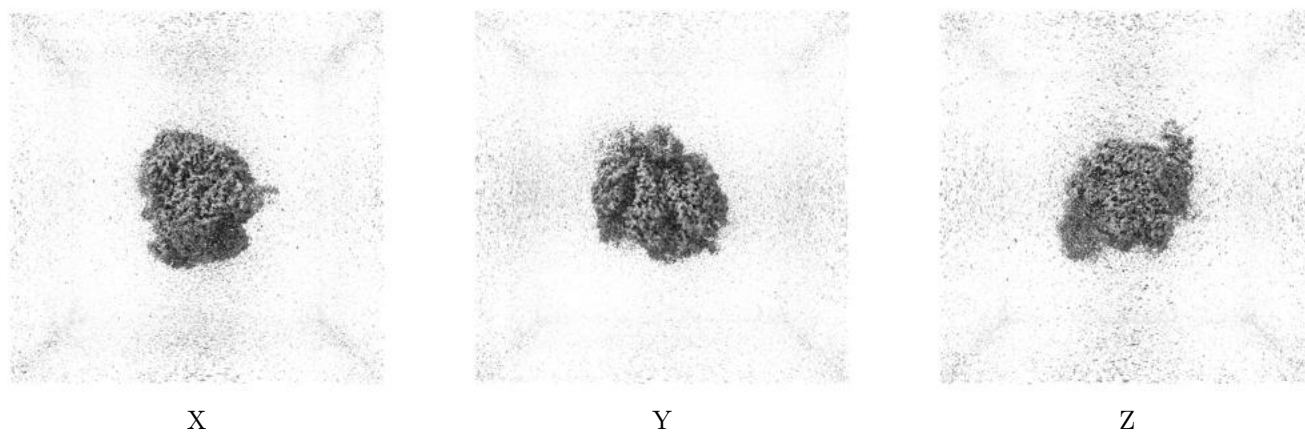
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

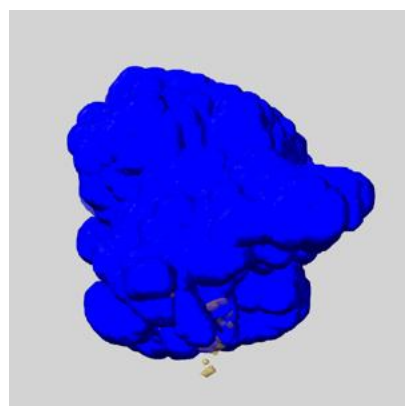
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

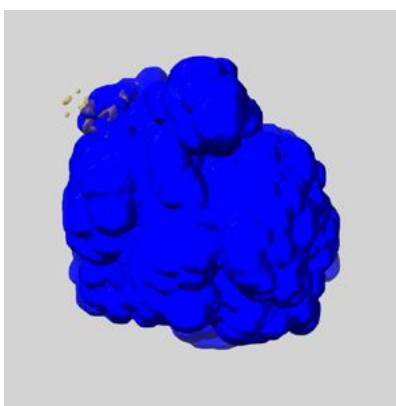
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

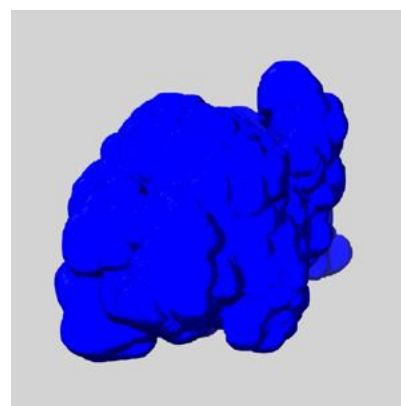
6.6.1 emd_66784_msk_1.map [i](#)



X



Y

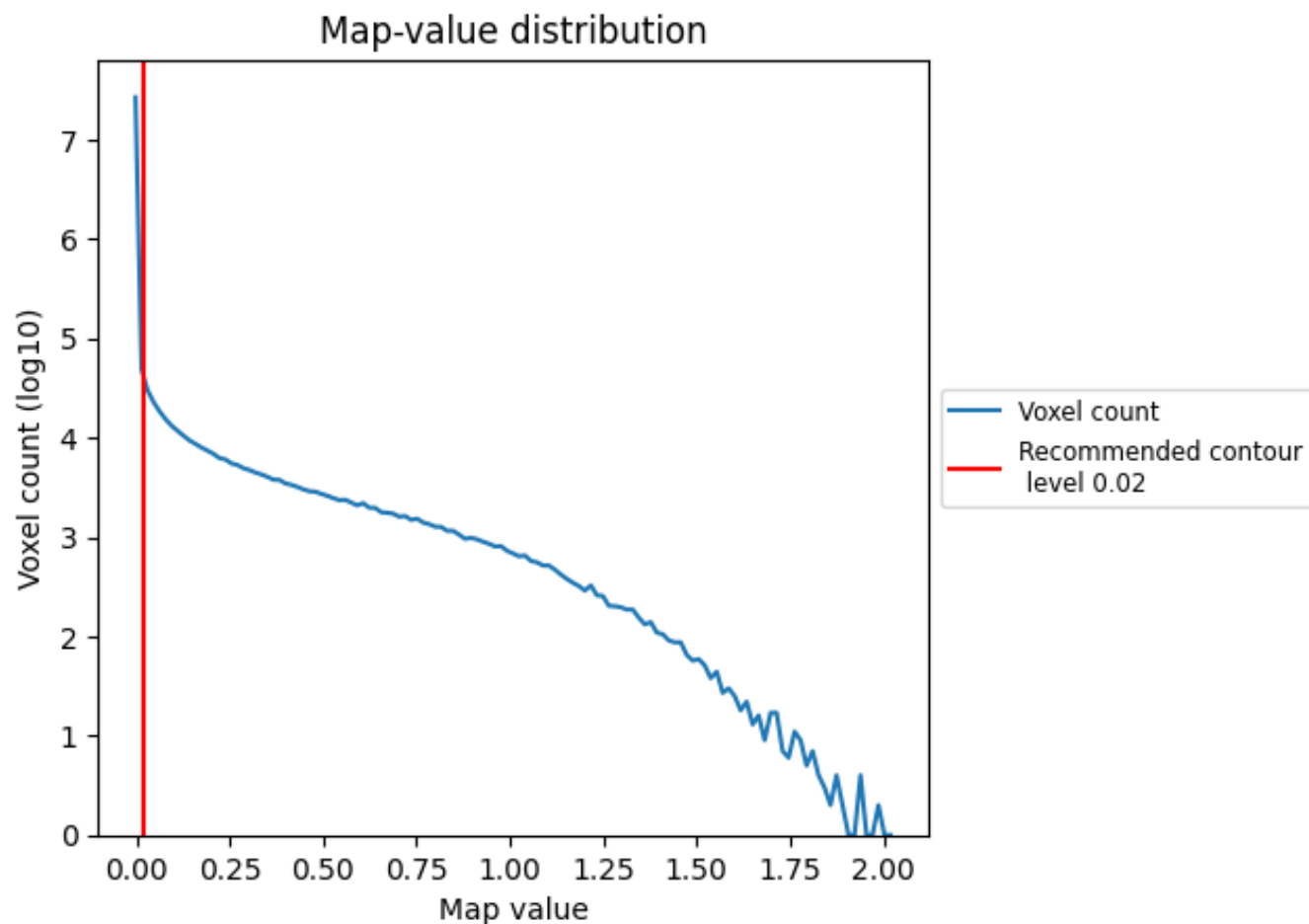


Z

7 Map analysis [i](#)

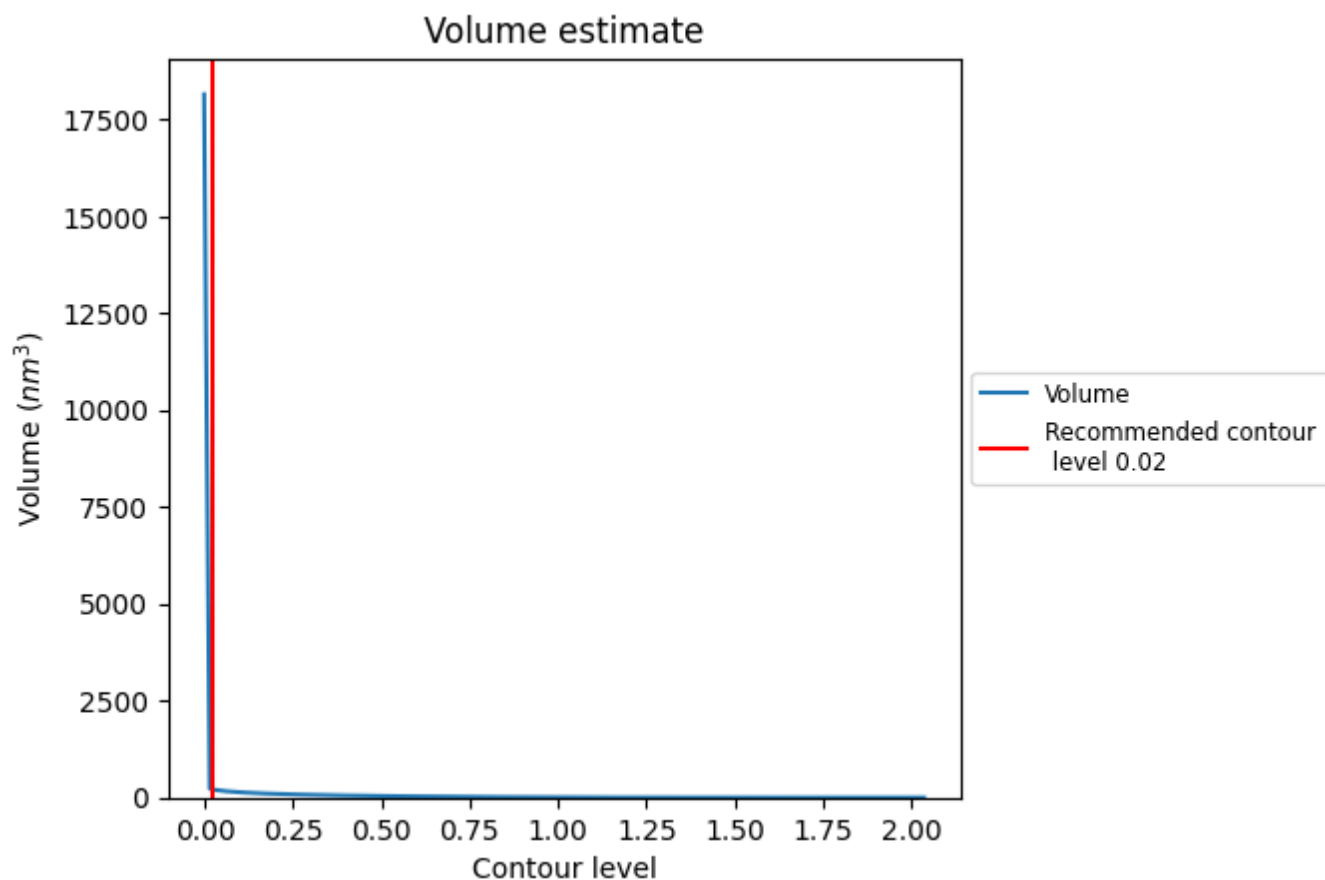
This section contains the results of statistical analysis of the map.

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.

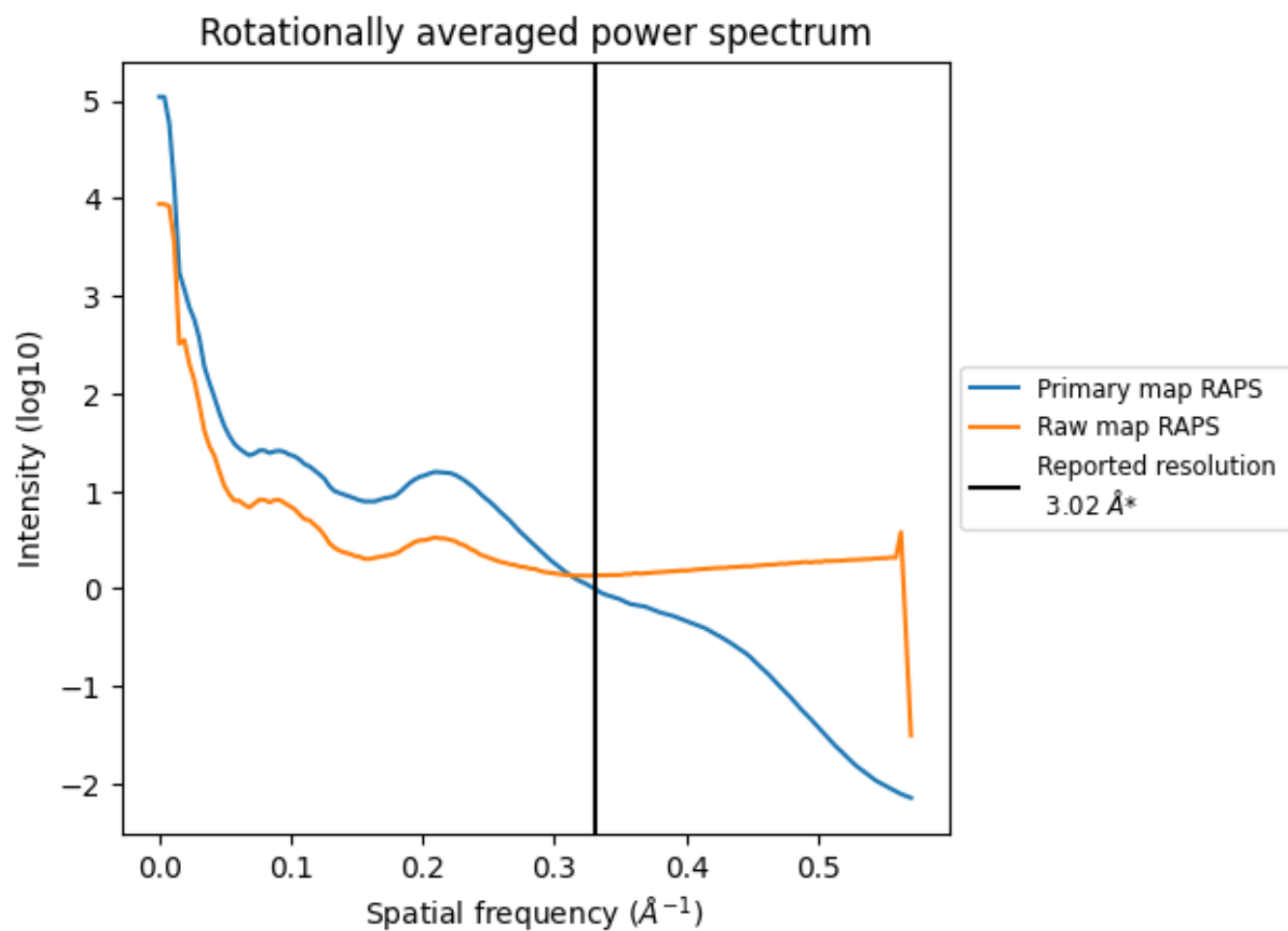
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 219 nm^3 ; this corresponds to an approximate mass of 197 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 ⓘ

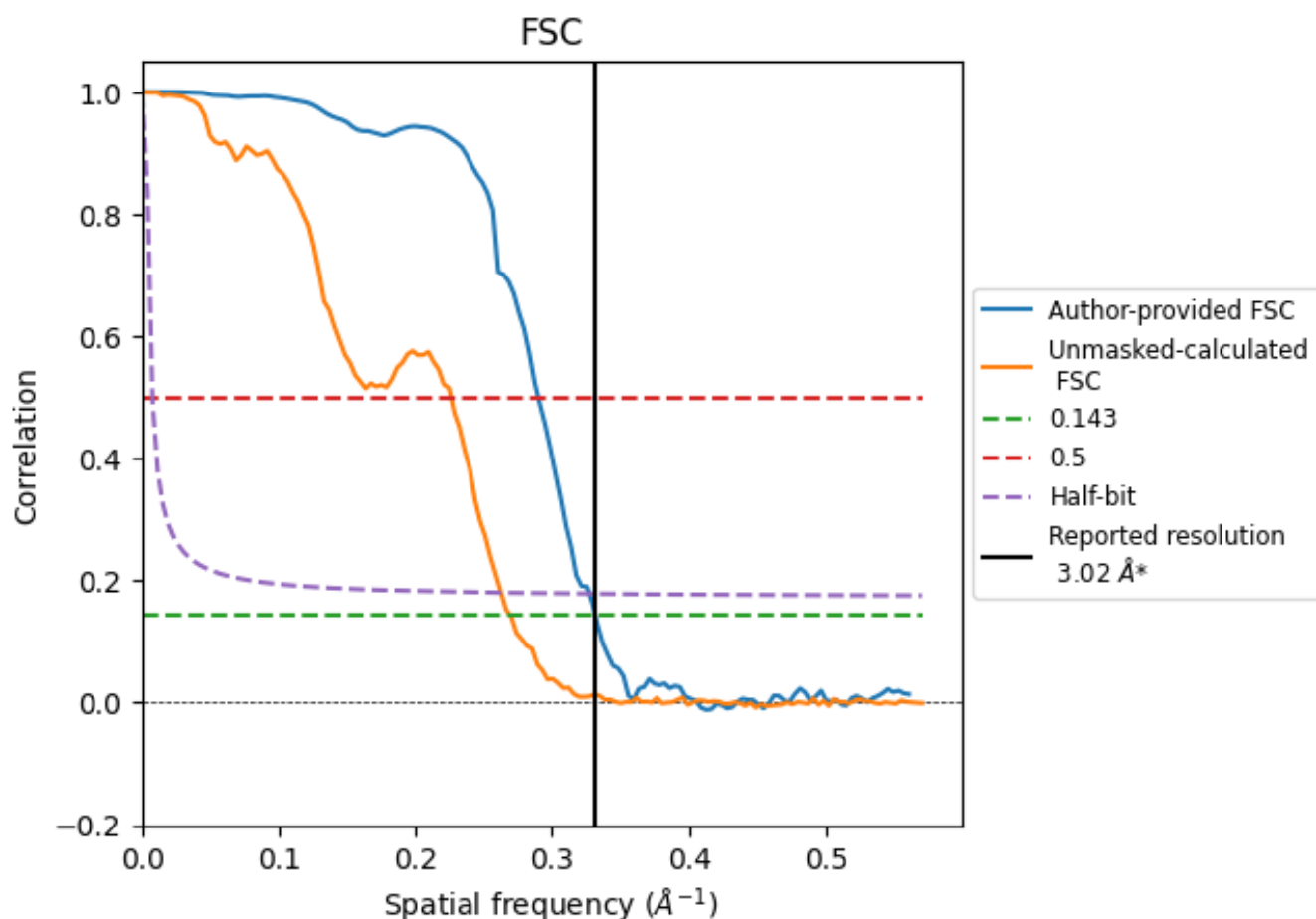


*Reported resolution corresponds to spatial frequency of 0.331 \AA^{-1}

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 0.331 \AA^{-1}

8.2 Resolution estimates [i](#)

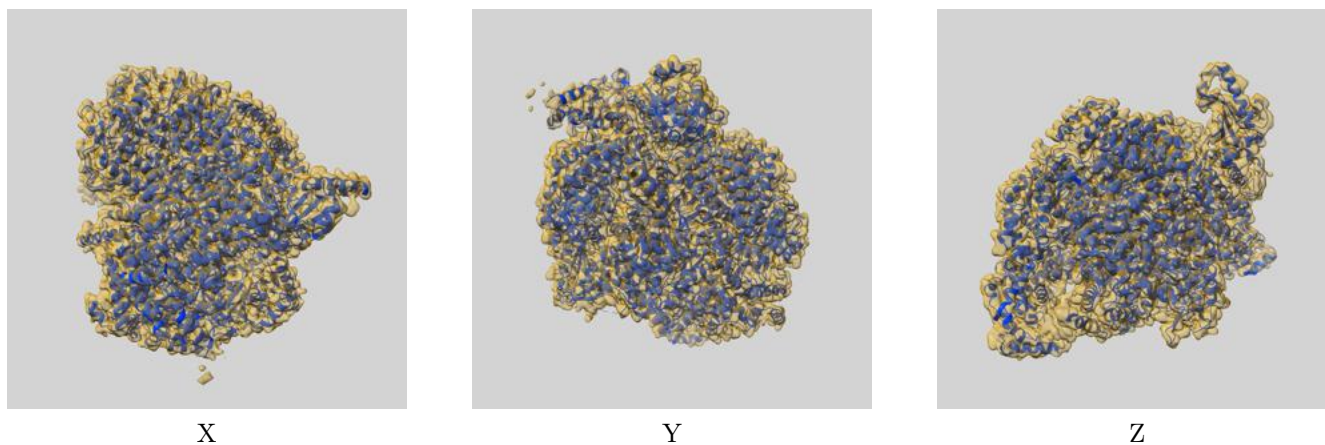
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.45	3.06
Unmasked-calculated*	3.71	4.43	3.81

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.71 differs from the reported value 3.02 by more than 10 %

9 Map-model fit [i](#)

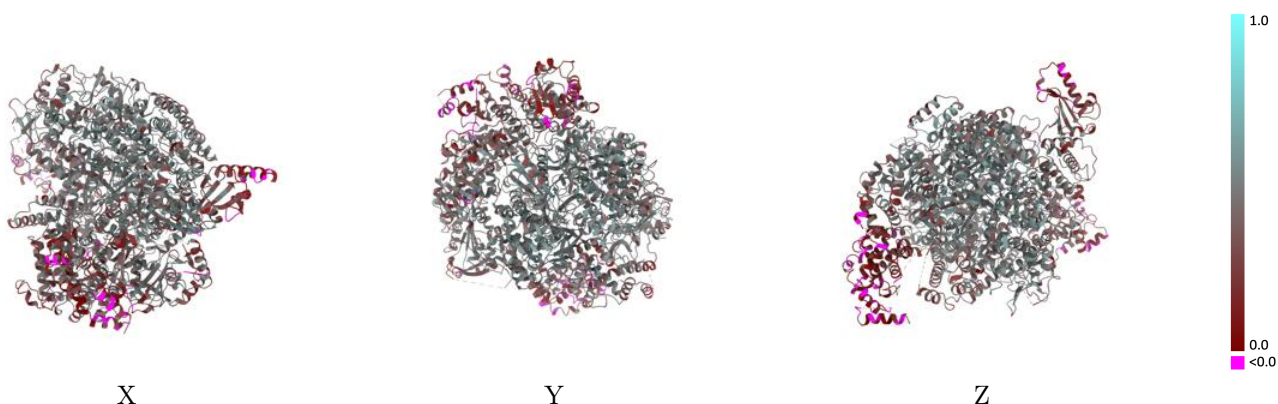
This section contains information regarding the fit between EMDB map EMD-66784 and PDB model 9XE7. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



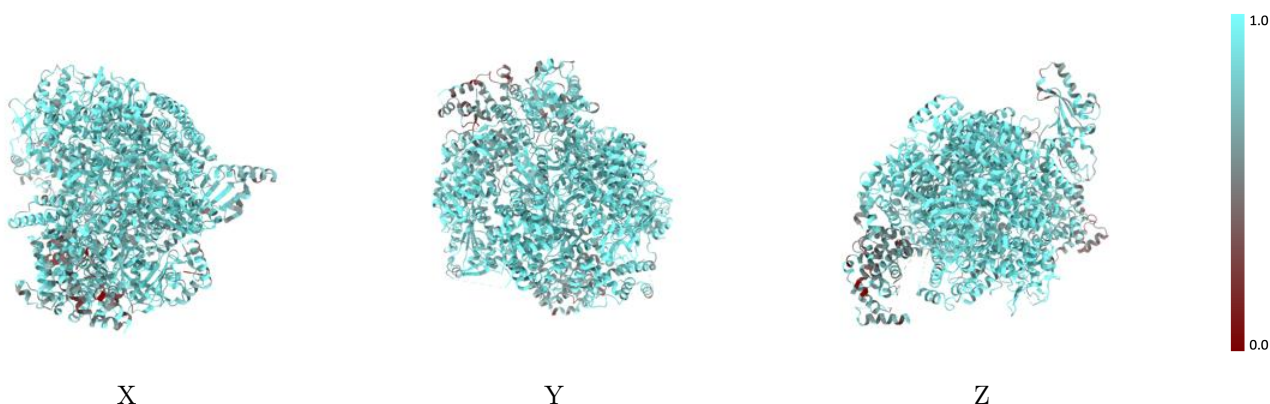
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



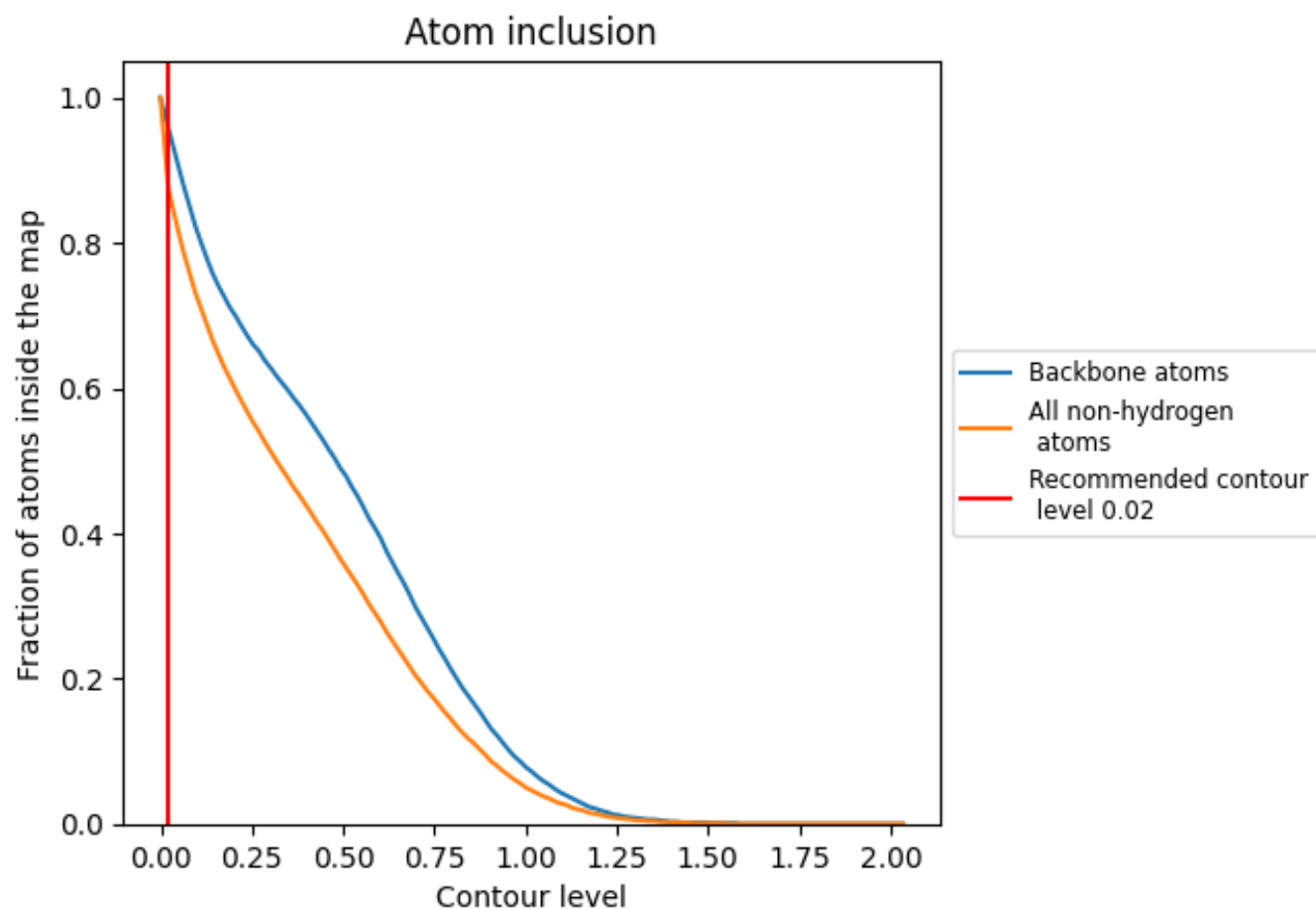
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 96% of all backbone atoms, 88% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8760	<div><div></div></div> 0.4080
A	<div><div></div></div> 0.8740	<div><div></div></div> 0.4070
B	<div><div></div></div> 0.9610	<div><div></div></div> 0.4740
C	<div><div></div></div> 0.9150	<div><div></div></div> 0.4120
D	<div><div></div></div> 0.9530	<div><div></div></div> 0.4630
E	<div><div></div></div> 0.9120	<div><div></div></div> 0.4370
F	<div><div></div></div> 0.9630	<div><div></div></div> 0.4620

1.0

0.0

<0.0