



wwPDB EM Validation Summary Report ⓘ

Feb 21, 2022 – 07:32 pm GMT

PDB ID : 7ORI
EMDB ID : EMD-13038
Title : La Crosse virus polymerase at replication late-elongation stage
Authors : Arragain, B.; Durieux Trouillette, Q.; Baudin, F.; Cusack, S.; Schoehn, G.;
Malet, H.
Deposited on : 2021-06-06
Resolution : 3.90 Å (reported)
Based on initial model : 6Z8K

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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

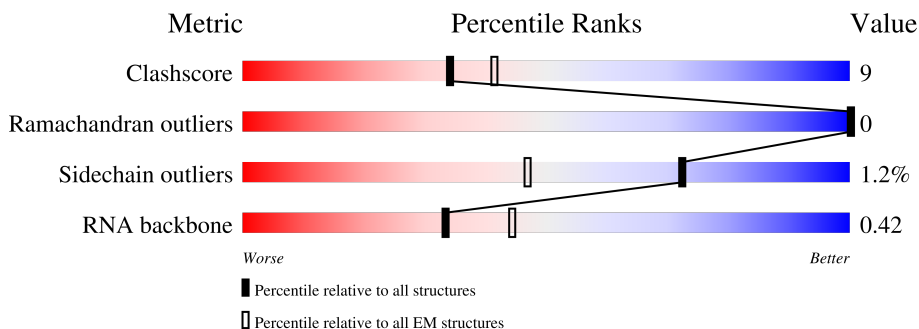
EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.26

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 3.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	H	17	18% (green), 35% (yellow), 12% (orange), 35% (grey)
2	T	30	13% (green), 47% (yellow), 10% (orange), 30% (grey)
3	P	30	10% (green), 27% (yellow), 60% (grey)
4	A	2276	69% (green), 19% (yellow), 12% (grey)

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17326 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 RNA chain called RNA (5'-R(P*AP*CP*GP*AP*GP*UP*GP*UP*CP*GP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	H	11	237	105	42	79	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	T	21	439	198	74	146	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	P	12	256	115	46	83	12	0	0

- Molecule 4 is a protein called La Crosse virus polymerase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	2007	16383	10499	2717	3059	108	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	LYS	HIS	engineered mutation	UNP A5HC98
A	1028G	SER	-	insertion	UNP A5HC98
A	1028H	GLY	-	insertion	UNP A5HC98
A	1028I	TRP	-	insertion	UNP A5HC98
A	1028J	SER	-	insertion	UNP A5HC98
A	1028K	HIS	-	insertion	UNP A5HC98

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1028L	PRO	-	insertion	UNP A5HC98
A	1028M	GLN	-	insertion	UNP A5HC98
A	1028N	PHE	-	insertion	UNP A5HC98
A	1028O	GLU	-	insertion	UNP A5HC98
A	1028P	LYS	-	insertion	UNP A5HC98
A	1028Q	GLY	-	insertion	UNP A5HC98
A	1028R	SER	-	insertion	UNP A5HC98
A	1028S	GLY	-	insertion	UNP A5HC98

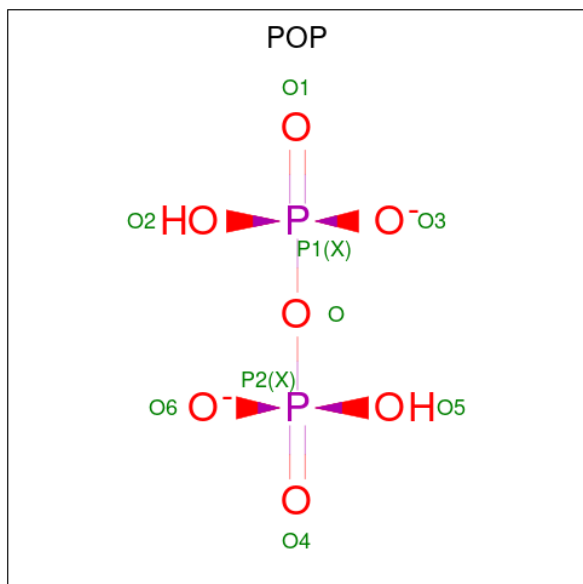
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Mg 1 1	0

- Molecule 7 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).

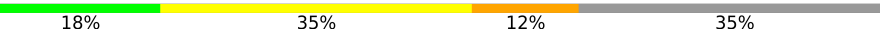


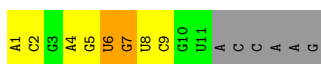
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total O P 9 7 2	0

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 (5'-R(P*AP*CP*GP*AP*GP*UP*GP*UP*CP*GP*U)-3')

Chain H: 



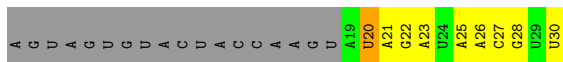
- Molecule 2: RNA (5'-R(P*AP*AP*CP*GP*UP*UP*AP*UP*CP*UP*AP*UP*AP*AP*CP*A P*CP*UP*AP*CP*U)-3')

Chain T: 



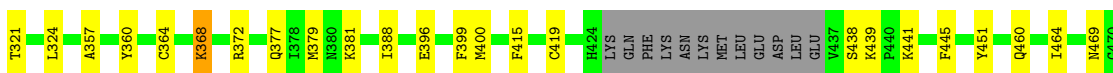
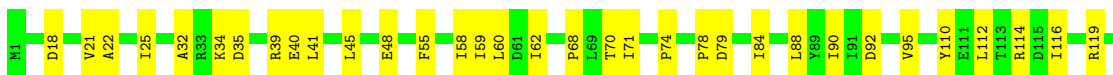
- Molecule 3: RNA (5'-R(P*AP*UP*AP*GP*AP*UP*AP*AP*CP*GP*UP*U)-3')

Chain P: 



- Molecule 4: La Crosse virus polymerase

Chain A: 



R2205	R2216	P2217	P2218	N2225	F2226	K2227	K2228	I2231	I2234	F2238	THR	THR	GLN	ASP	PHE	ASP	N2134	G2135	F2136	N2141	L2145	V2148	V2149	L2152	N2160	F2160	R2161	L2166	H2169	L2172	M2177	D2178	H2179	Y2181	F2184	D2185	F2190	MET	GLY	ASN	PRO	ILE	THR	ARG	ASP	I2199			
K643	R653	Y794	V794	L796	K797	I798	L799	K805	R813	L817	R868	L869	F695	Y710	L711	I716	I717	Q718	K719	G720	I721	N724	I730	W731	F732	V736	T737	L738	Y746	L747	P748	F751	K754	M763	L766	A767	K768	L771	I772	E773	E774	N780	I781						
K782	V794	W794	V794	L796	K797	I798	L799	K805	R813	L817	R868	L869	F695	Y710	L711	I716	I717	Q718	K719	G720	I721	N724	I730	W731	F732	V736	T737	L738	Y746	L747	P748	F751	K754	M763	L766	A767	K768	L771	I772	E773	E774	N780	I781						
CYS	ASN	Y893	R897	Y906	Y929	K933	M934	Y937	Y944	F947	K950	G951	Q952	R958	F959	I960	F961	K968	N969	C970	K979	E980	N981	C982	K983	L984	N985	P986	D987	E988	L998	K999	R1017	Q1018	K1019	N1020	R1021	D1024	I1027	E1028	ALA	LEU	LEU	THR					
GLU	GLY	GLY	SER	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	SER	GLY	TYR	GLU	SER	ASN	LEU	GLY	I1042	E1043	K1044	L1045	S1046	K1049	A1050	A1059	D1060	W1064	S1065	A1066	W1075	R1090	Y1093	L1103	I1104	L1105	P1106	Y1120	D1123	A1126	T1127	M1128	Q1131	W1143			
L1144	Q1145	G1146	M1147	F1148	N1149	Y1150	T1151	S1152	K1164	E1165	K1168	E1169	A1170	I1171	T1172	L1173	L1174	I1178	D1188	I1195	D1198	T1232	I1235	K1236	L1241	F1242	N1243	L1244	I1251	R1254	F1255	L1256	D1271	L1272	A1273	S1274	R1275	I1276	S1277	K1284	P1289	W1293	V1294	S1295					
I1298	P1317	A1323	R1326	K1327	D1328	K1340	L1341	S1342	M1343	T1346	I1347	G1348	L1349	L1354	L1357	I1358	K1359	L1360	T1365	R1371	S1372	S1373	Q1377	I1378	K1382	T1390	E1393	K1398	R1401	Y1402	L1403	D1406	A1407	M1409	T1418	S1419	D1420	M1421	V1422	G1423									
R1424	R1439	L1441	E1466	K1467	L1498	A1504	F1507	I1508	I1511	L1511	V1516	F1517	V1518	Y1528	P1642	T1643	E1644	M1645	A1646	R1647	H1651	K1666	V1667	R1668	M1671	K1686	R1690	Q1693	Y1696	E1697	Y1698	V1699	K1700	S1701	T1702	F1709	S1715	T1718	L1724	L1729									
I1730	K1731	Y1736	Q1743	L1744	L1745	S1759	E1760	A1764	C1767	F1768	K1769	L1770	L1771	L1772	H1773	L1790	I1791	E1794	F1795	S1796	Y1797	L1805	Y1813	P1820	L1828	R1829	L1833	D1837	K1840	SER	HIS	Y1699	K1700	S1701	T1702	F1709	S1715	T1718	L1724	L1729									
ASP	MET	GLY	SER	ILE	ASN	THR	THR	TYR	ARG	SER	LYS	THR	ILE	GLY	GLU	ASP	ASN	LYS	THR	ALA	ASP	SER	ARG	ALA	LEU	LYS	PRO	GLU	ASN	ILE	THR	THR	GLY	ARG	LYS	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	
LYS	ILE	GLN	THR	TYR	PRO	GLY	ASN	TYR	ARG	SER	LYS	THR	ILE	GLY	GLU	ASP	ASN	LYS	THR	ALA	ASP	SER	ARG	ALA	LEU	LYS	PRO	GLU	ASN	ILE	THR	THR	GLY	ARG	LYS	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	GLY	ASP	ARG	I1982	L1987	S1998	R1999	I2000	T2009	I2010	K2011	K2012	G2023	P2024	L2030	T2034	E2035	K2038	S2039	N2046	N2049	F2050	R2051	L2055	I2062	C2063	C2064	N2071	D2072	P2081	T2085	E2086	G2087	I2090	H2091	S2092	T2093	P2094	T2095	F2096	H2097	I2098	Y2099						
Y2100	S2101	R2102	R2103	L2116	L2117	I2118	E2119	R2120	E2121	T2122	E2126	E2127	A2128	F2129	T2130	F2134	G2135	F2136	N2141	L2145	V2148	V2149	L2152	W2160	K2166	H2169	L2172	M2177	D2178	H2179	Y2181	F2184	D2185	F2190	MET	GLY	ASN	PRO	ILE	THR	ARG	ASP	I2199						
R2205	I2216	P2217	P2218	N2225	F2226	K2227	K2228	I2231	I2234	F2238	THR	THR	GLN	ASP	PHE	ASP	N2134	G2135	F2136	N2141	L2145	V2148	V2149	L2152	W2160	K2166	H2169	L2172	M2177	D2178	H2179	Y2181	F2184	D2185	F2190	MET	GLY	ASN	PRO	ILE	THR	ARG	ASP	I2199					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24151	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	297.69998, 297.69998, 297.69998	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.145, 1.145, 1.145	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: POP, ZN, MG

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	H	0.69	1/264 (0.4%)	0.67	0/408
2	T	0.22	0/488	0.79	0/753
3	P	0.23	0/286	0.72	0/443
4	A	0.27	0/16721	0.45	0/22547
All	All	0.28	1/17759 (0.0%)	0.48	0/24151

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	1	A	OP3-P	-10.66	1.48	1.61

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	H	237	0	119	4	0
2	T	439	0	226	14	0
3	P	256	0	129	10	0
4	A	16383	0	16426	289	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	9	0	0	0	0
All	All	17326	0	16900	305	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 9.

The worst 5 of 305 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)
4:A:813:ARG:NH1	4:A:986:PRO:HD3	1.67	1.09
4:A:2064:CYS:HB2	4:A:2169:HIS:HE1	1.15	1.03
4:A:2064:CYS:CB	4:A:2169:HIS:HE1	1.76	0.98
4:A:2064:CYS:HB2	4:A:2169:HIS:CE1	1.97	0.98
4:A:813:ARG:HH12	4:A:986:PRO:HD3	1.35	0.89

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
4	A	1991/2276 (88%)	1923 (97%)	68 (3%)	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
4	A	1852/2097 (88%)	1829 (99%)	23 (1%)	71 83

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	1390	THR
4	A	2051	ARG
4	A	1602	ARG
4	A	2072	ASP
4	A	655	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	622	ASN
4	A	760	HIS
4	A	1580	ASN
4	A	1704	HIS
4	A	1743	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	H	10/17 (58%)	4 (40%)	0
2	T	19/30 (63%)	9 (47%)	0
3	P	11/30 (36%)	1 (9%)	0
All	All	40/77 (51%)	14 (35%)	0

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	H	6	U
1	H	7	G
1	H	8	U
1	H	9	C
2	T	2	A

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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	$\# Z > 2$
7	POP	A	2303	-	6,8,8	0.80	0	13,13,13	0.74	0

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
7	POP	A	2303	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

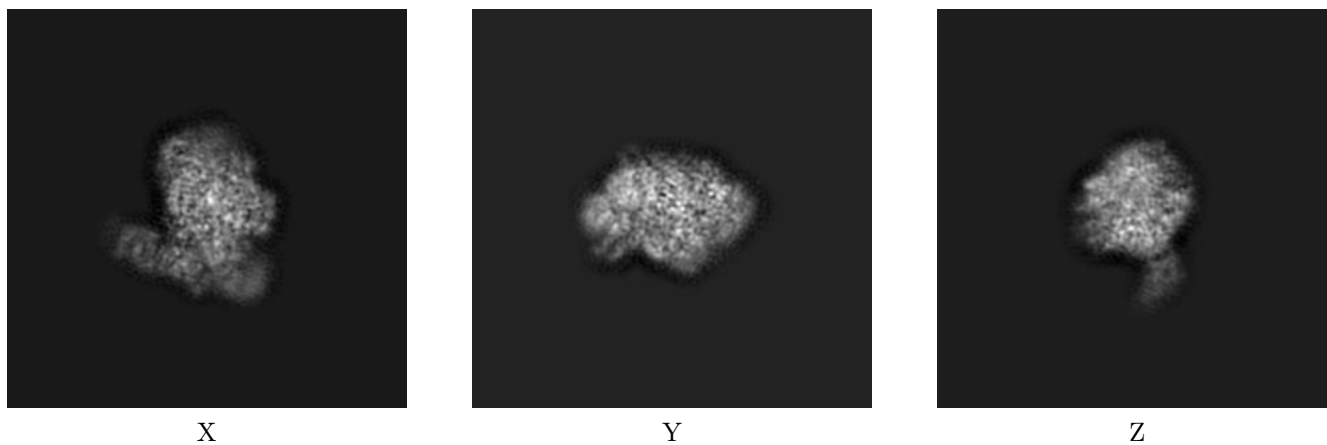
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13038. 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](#)

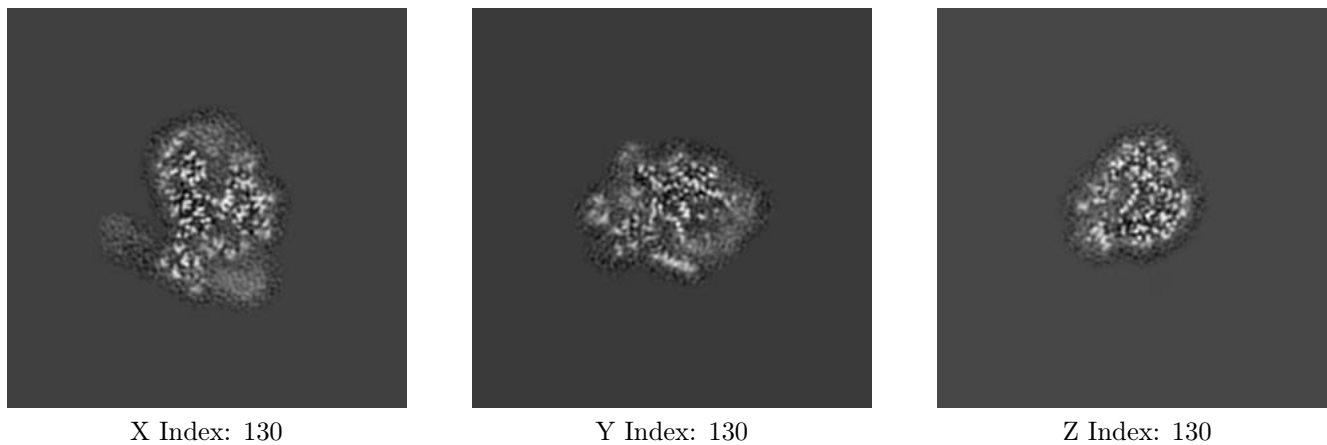
6.1.1 Primary map



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

6.2 Central slices [i](#)

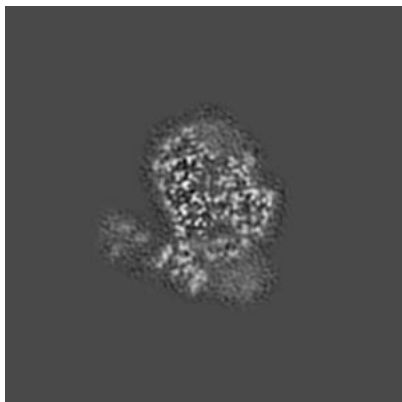
6.2.1 Primary map



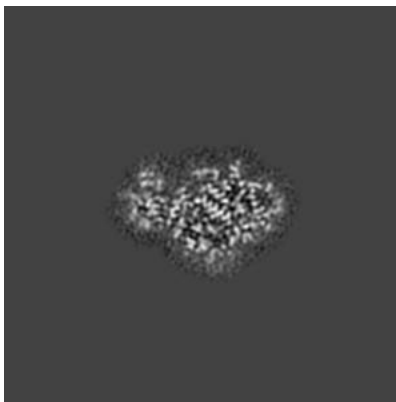
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

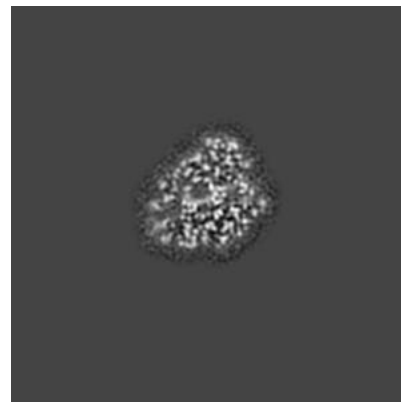
6.3.1 Primary map



X Index: 133



Y Index: 116



Z Index: 134

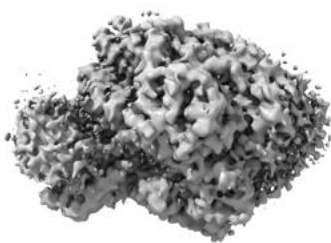
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

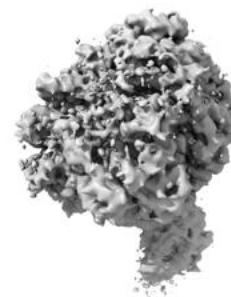
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

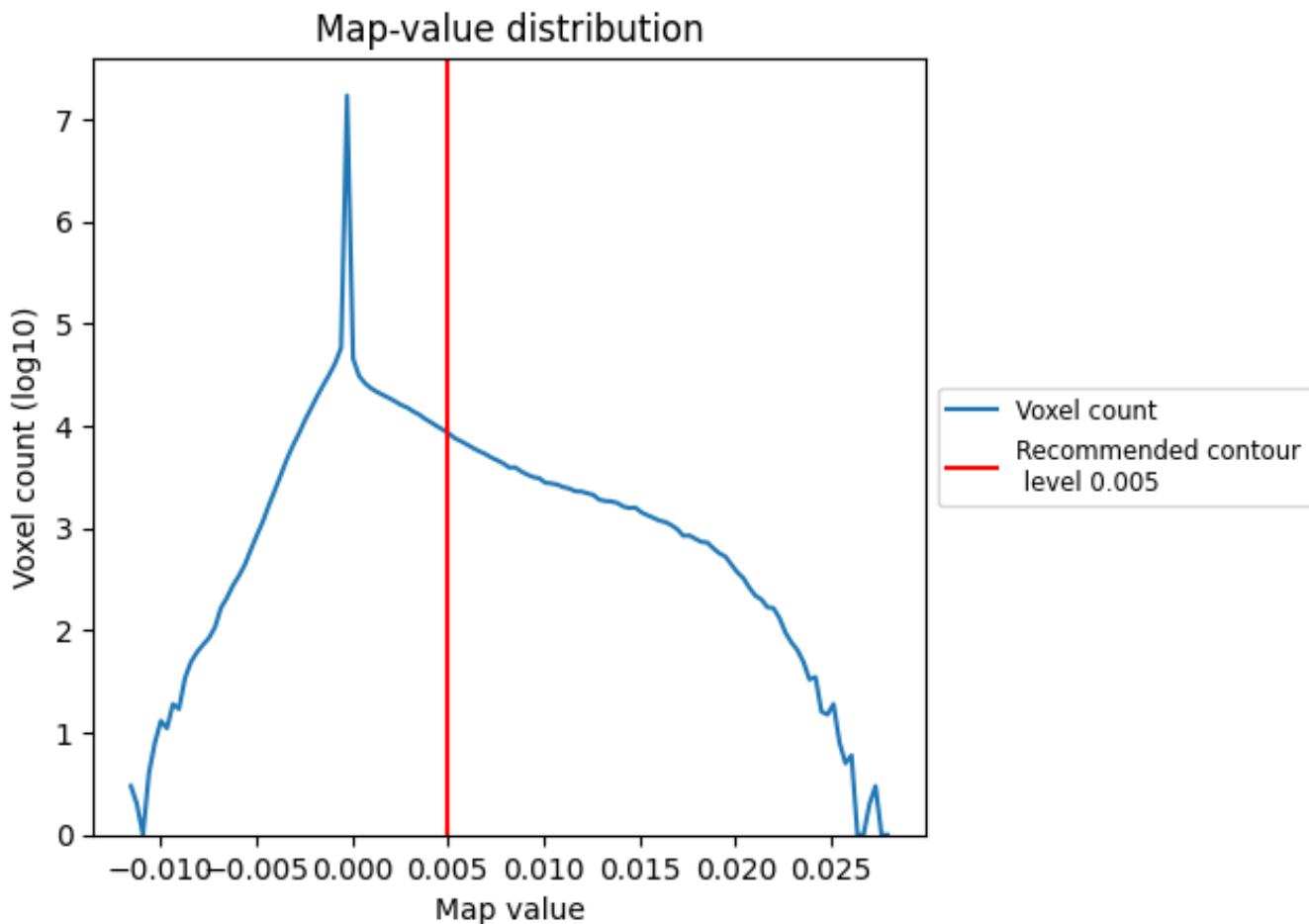
6.5 Mask visualisation

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

7 Map analysis [i](#)

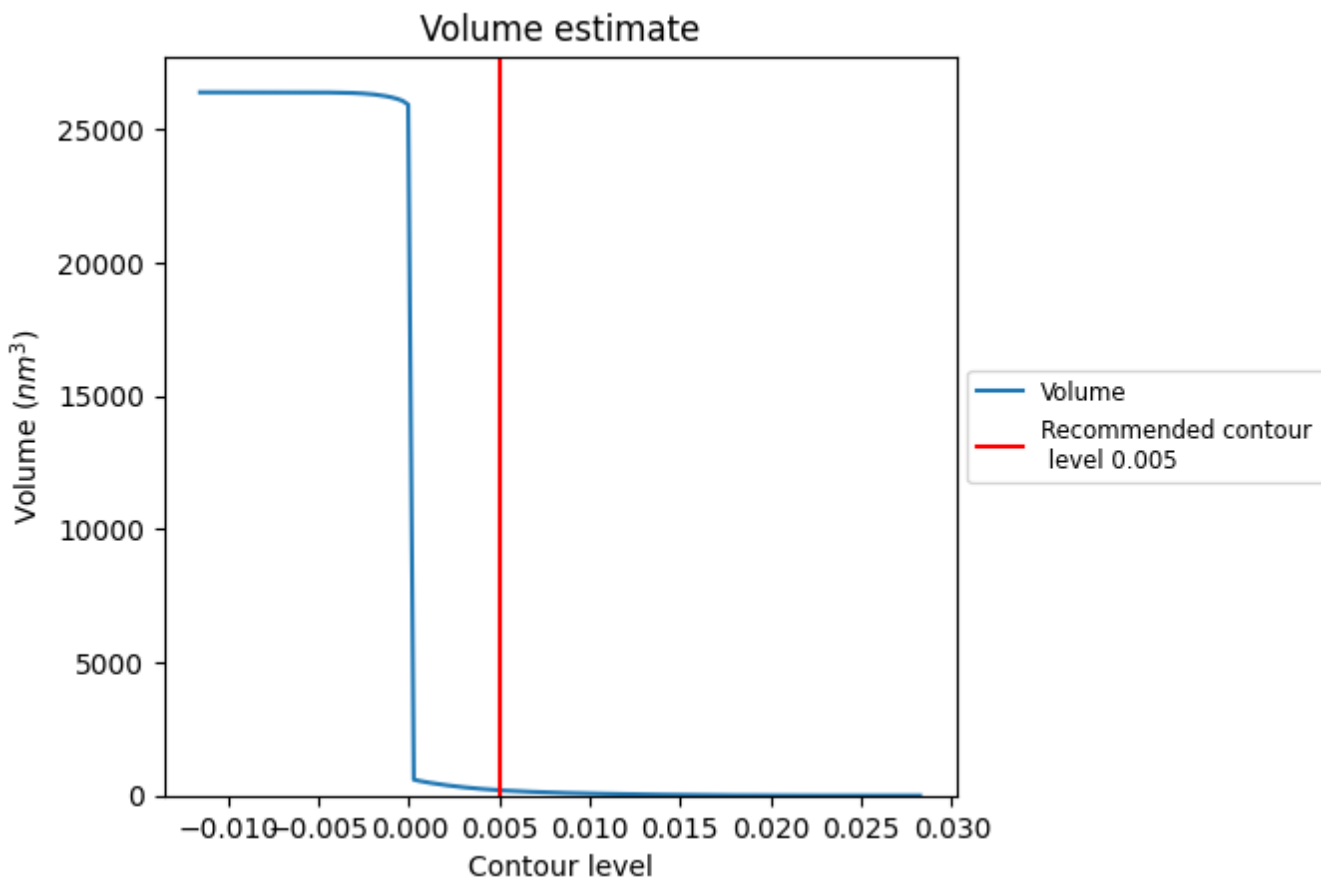
This section contains the results of statistical analysis of the map.

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.

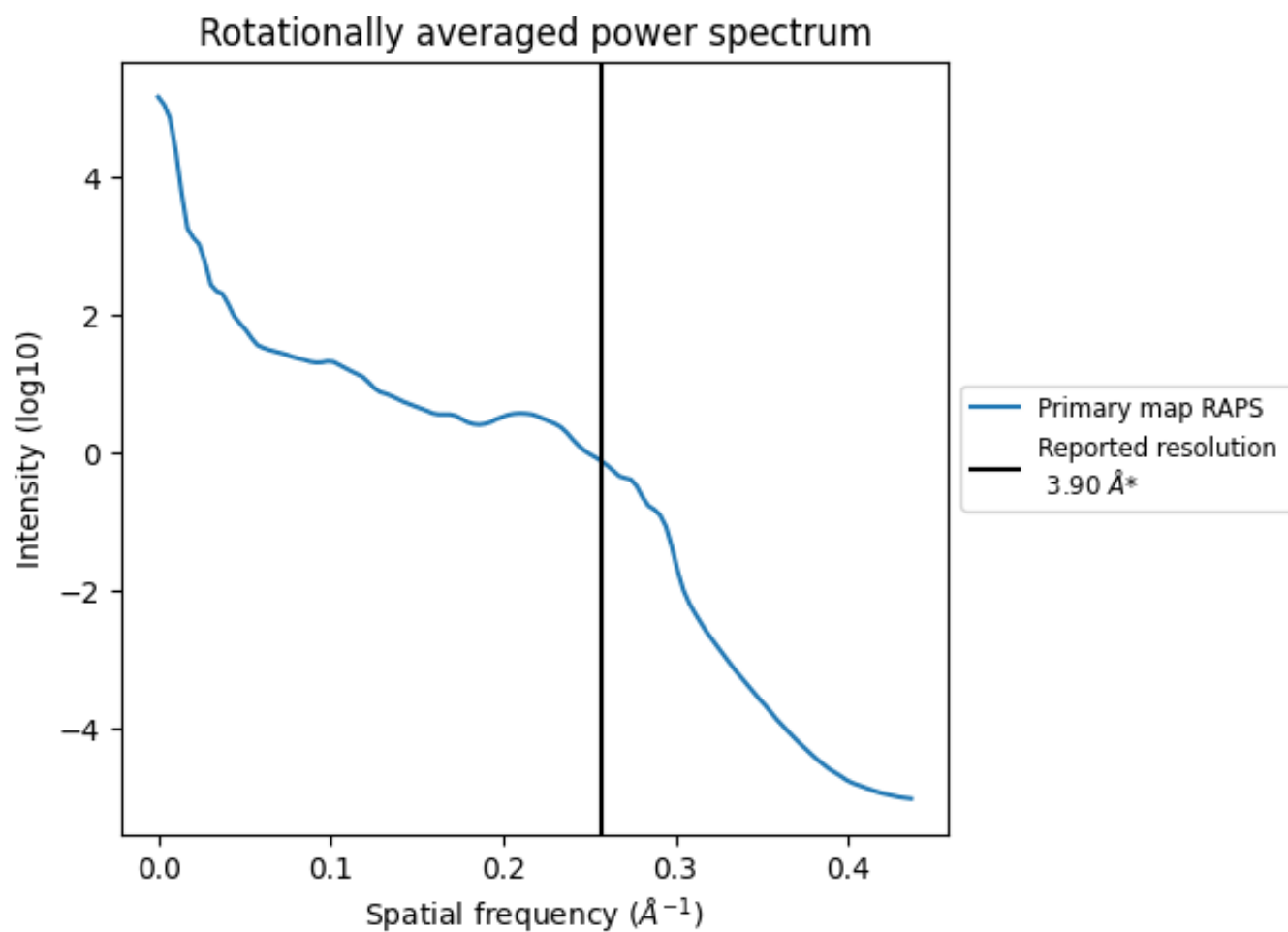
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 201 nm³; this corresponds to an approximate mass of 182 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 [i](#)

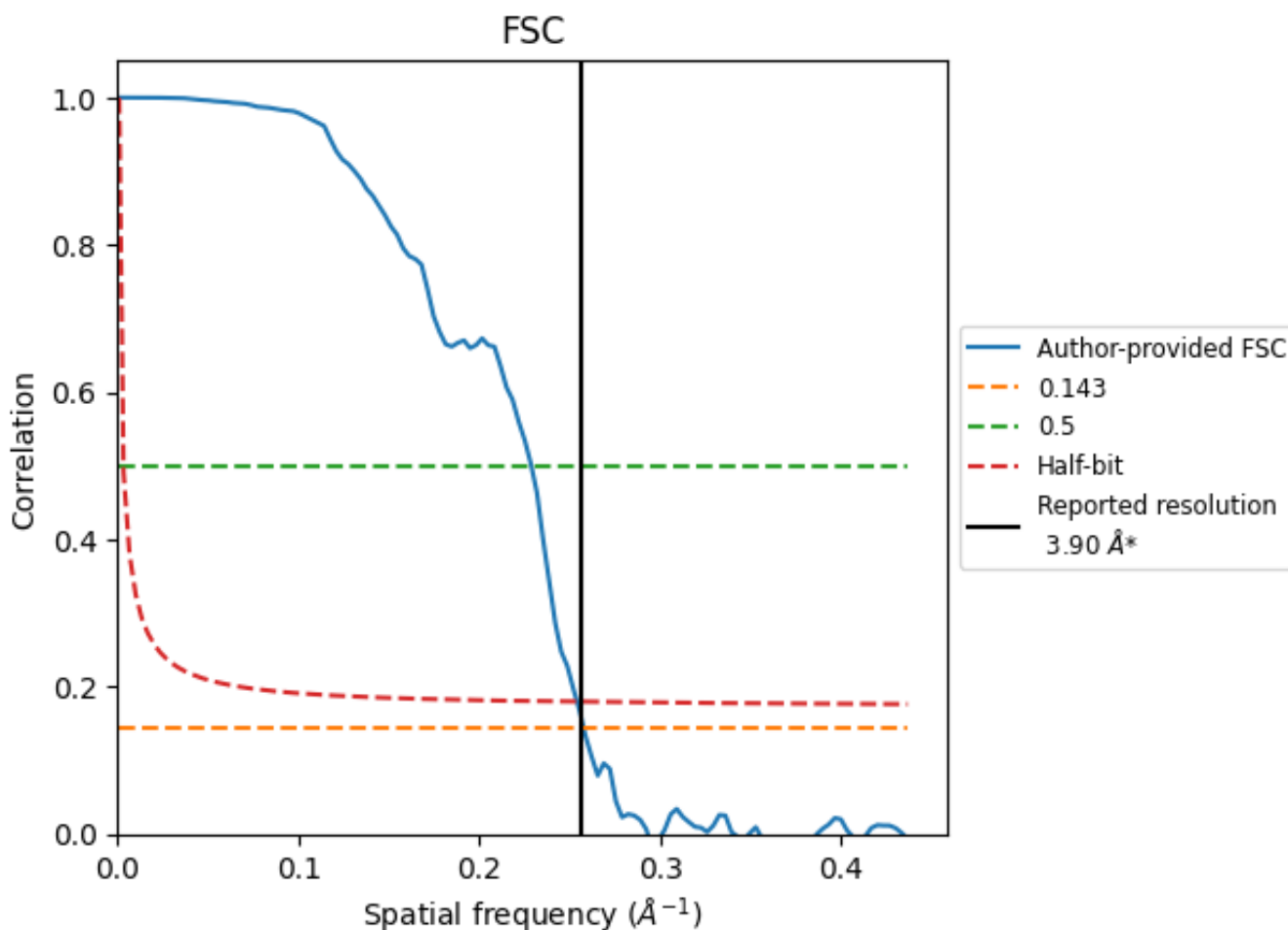


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

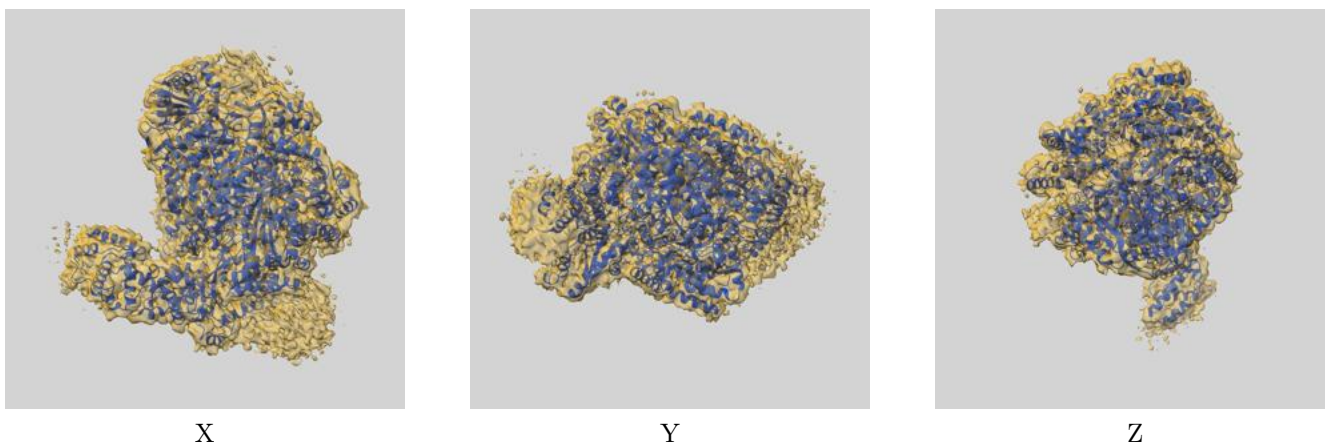
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.88	4.37	3.94
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

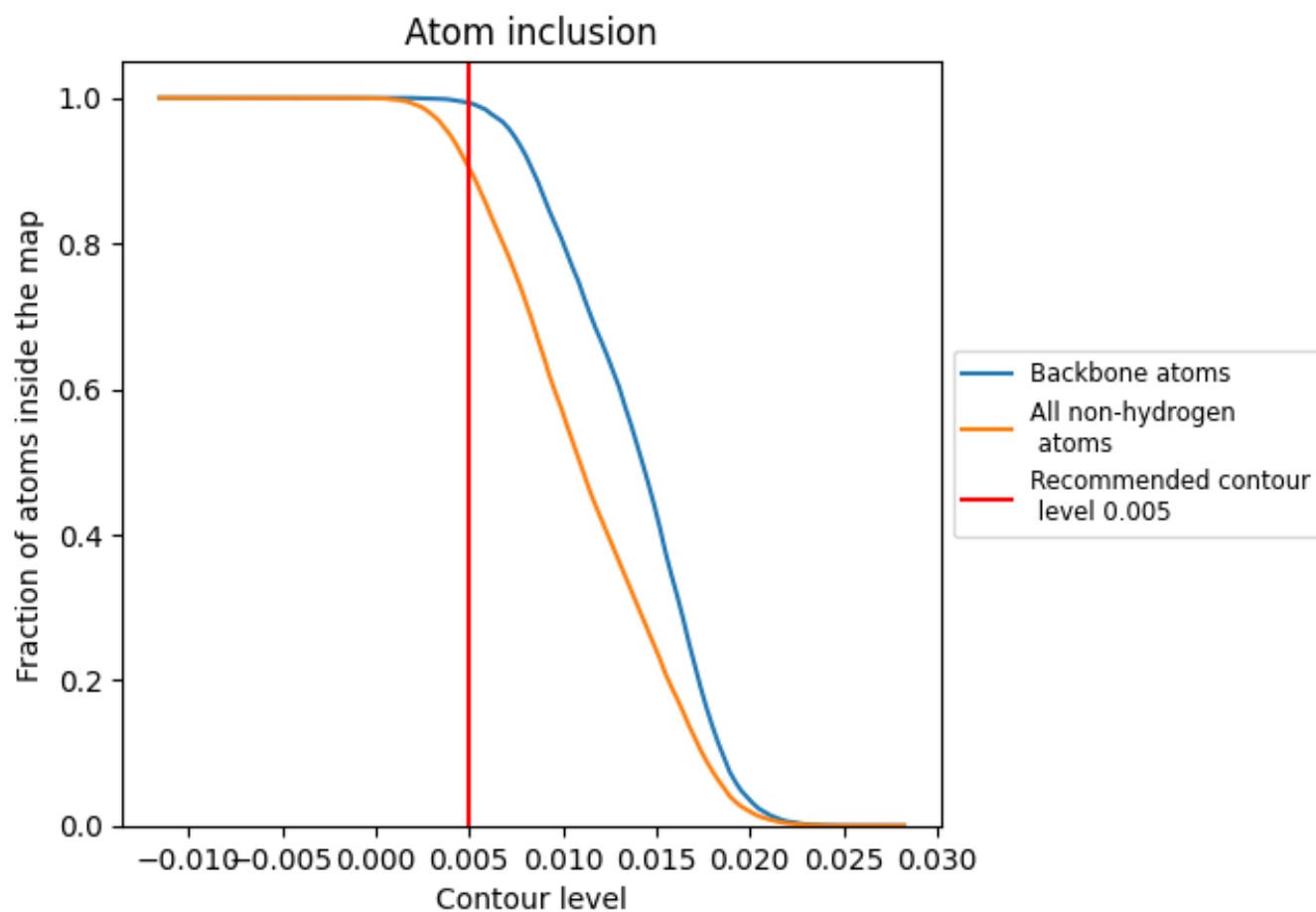
This section contains information regarding the fit between EMDB map EMD-13038 and PDB model 7ORI. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.005 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 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.