



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2022 – 06:23 am GMT

PDB ID : 7QXS
EMDB ID : EMD-14197
Title : Cryo-EM structure of human telomerase-DNA-TPP1-POT1 complex (with POT1 side chains)
Authors : Sekne, Z.; Ghanim, G.E.; van Roon, A.M.M.; Nguyen, T.H.D.
Deposited on : 2022-01-27
Resolution : 3.91 Å (reported)
Based on initial models : 1XJV, 7BG9

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:

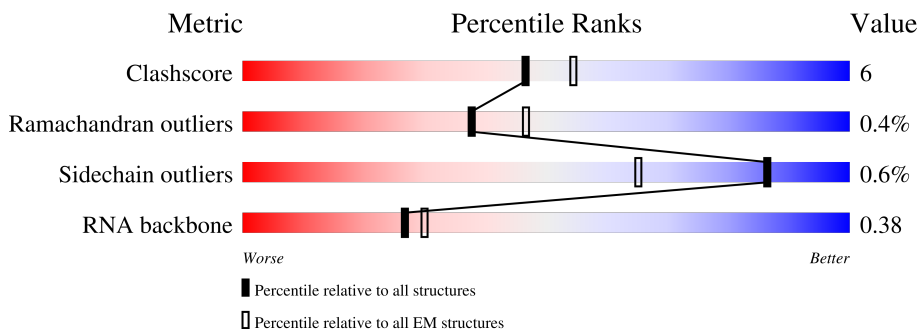
EMDB validation analysis : 0.0.0.dev97
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

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 3.91 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	A	1132	
2	B	451	
3	L	130	
4	M	166	
5	N	30	
6	O	458	
7	P	634	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17820 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 Telomerase reverse transcriptase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	951	7626	4892	1418	1280	36	0	0

- Molecule 2 is a RNA chain called RNA (256-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	256	5431	2420	947	1808	256	0	0

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	L	82	643	403	128	112	0	0

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	90	699	440	123	134	2	0	0

- Molecule 5 is a DNA chain called Telomeric DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	N	22	461	220	86	134	21	0	0

- Molecule 6 is a protein called Adrenocortical dysplasia homolog (Mouse), isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	O	120	955	603	171	177	4	0	0

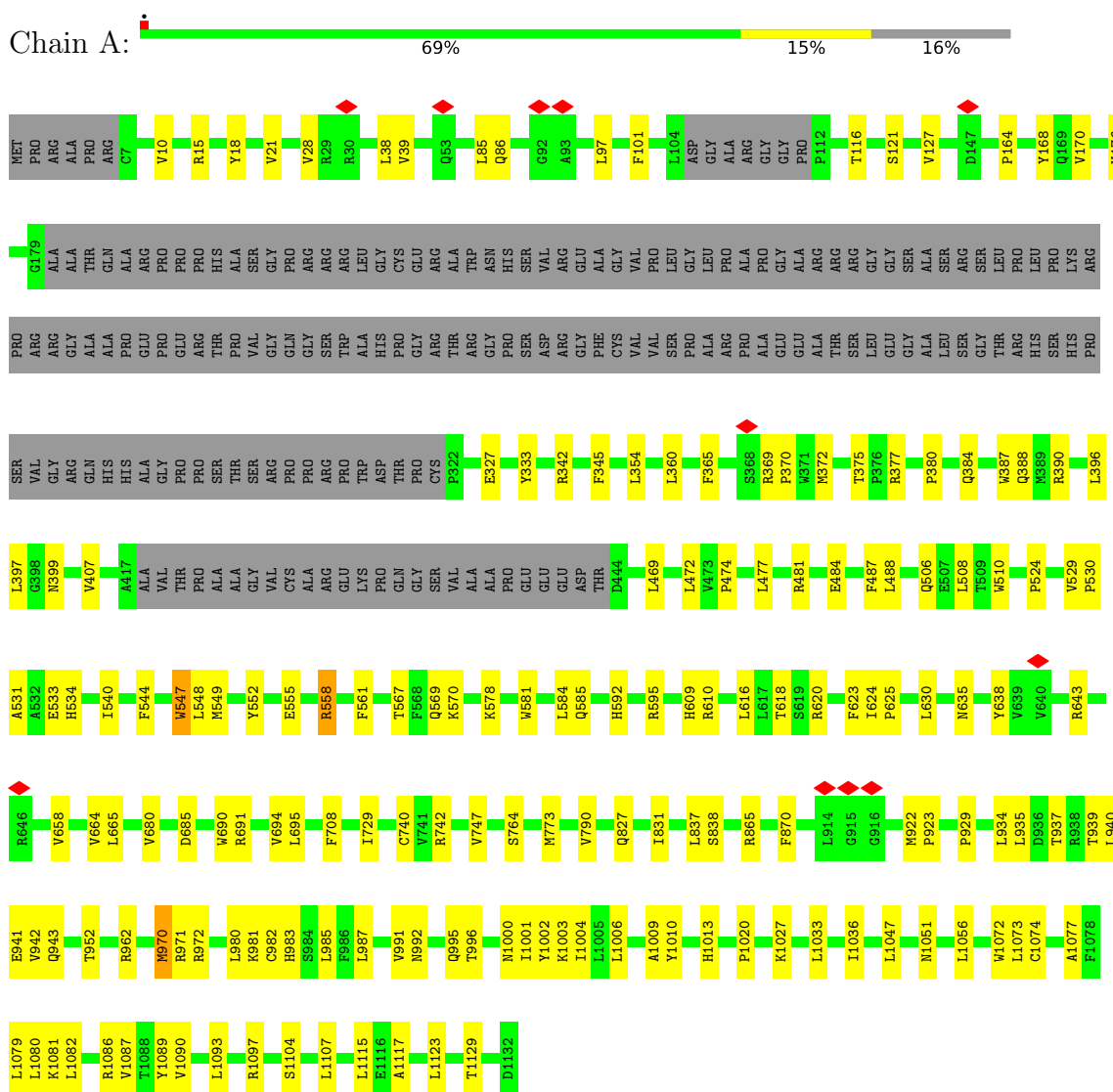
- Molecule 7 is a protein called Protection of telomeres protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	P	251	2005	1299	337	364	5	0	0

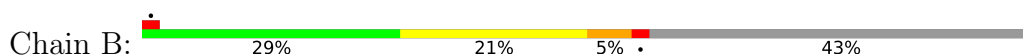
3 Residue-property plots [\(i\)](#)

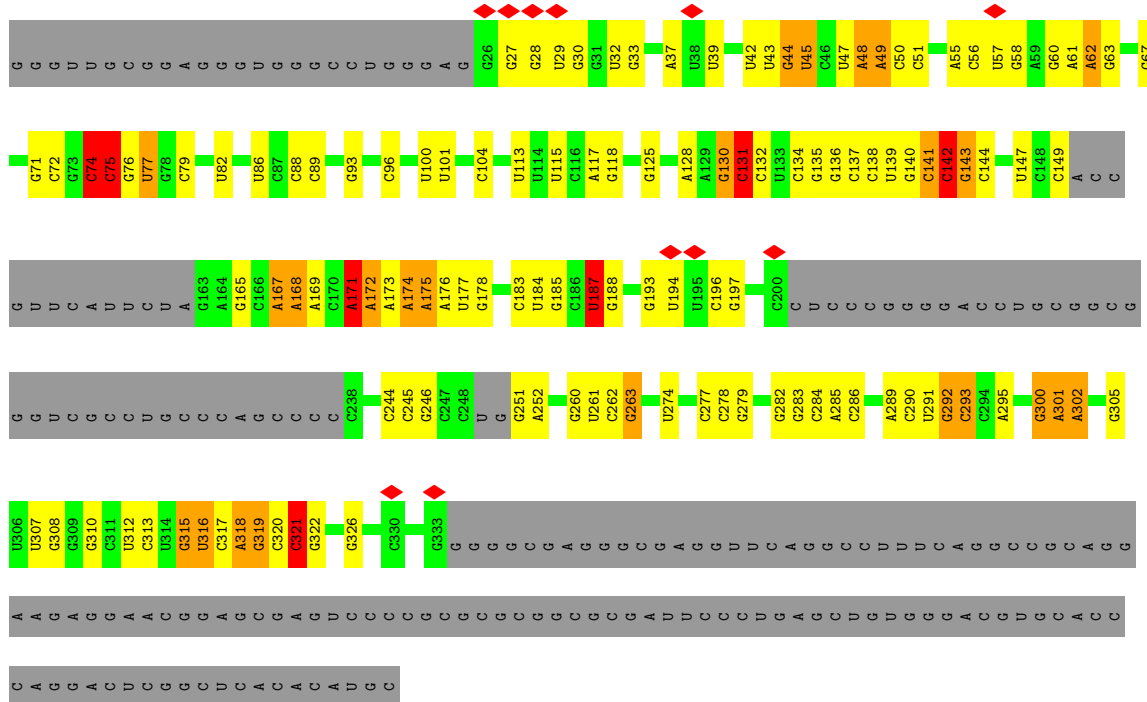
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Telomerase reverse transcriptase

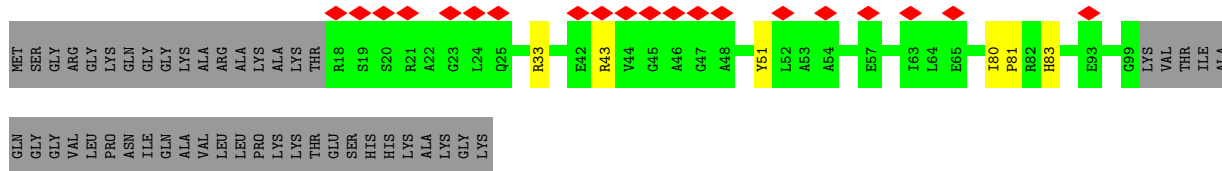


• Molecule 2: RNA (256-MER)

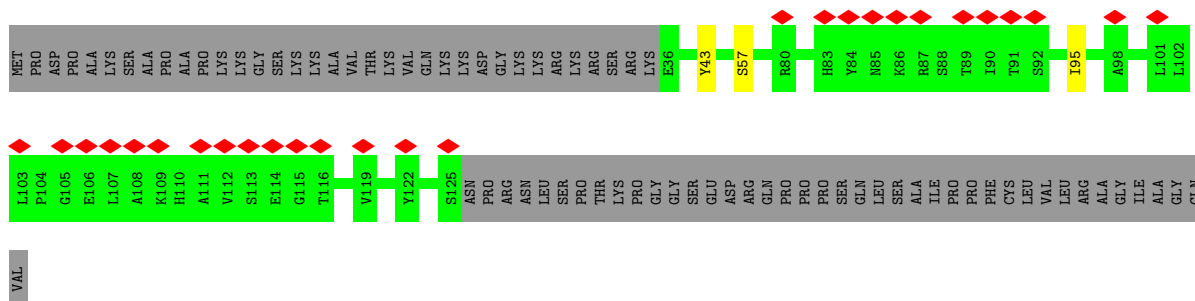




• Molecule 3: Histone H2A



• Molecule 4: Histone H2B



• Molecule 5: Telomeric DNA



LYS VAL
LEU ILE
GLN ALA
VAL GLY
THR HIS
PHE THR
VAL PHE
LYS VAL
ASN ASN
GLY GLY
ILE ILE
LEU LEU
PRO PRO
LEU LEU
SER SER
LEU LEU
ASN ASN
GLU GLU
CYS CYS
LEU LEU
LEU LEU
LEU LEU
ILE ILE
GLN GLN
ASN ASN
ASN ASN
SER SER
LEU LEU
ARG ARG
GLU GLU
CYS CYS
LEU LEU
LEU LEU
GLN GLN
ASN ASN
LEU LEU
ILE ILE
SER SER
LEU LEU
VAL VAL
ASP ASP
LYS LYS
THR THR
SER SER
ILE ILE
TRP TRP
ILE ILE
PRO PRO
SER SER
SER SER
ASN ASN
VAL VAL
ALA ALA
GLU GLU
SER SER
ALA ALA
LEU LEU
GLY GLY
ILE ILE
PRO PRO
VAL VAL
ARG ARG

LEU ILE
GLN ALA
THR HIS
ILE ILE
HIS HIS
TYR TYR
GLY GLY
CYS CYS
LYS LYS
GLN GLN
CYS CYS
SER SER
SER SER
LEU LEU
ARG ARG
SER SER
ILE ILE
GLN GLN
ASN ASN
LEU LEU
ASN ASN
SER SER
LEU LEU
VAL VAL
TRP TRP
ILE ILE
PRO PRO
SER SER
SER SER
ASN ASN
VAL VAL
ALA ALA
GLU GLU
SER SER
ALA ALA
LEU LEU
GLY GLY
ILE ILE
VAL VAL
PRO PRO
ARG ARG
LEU LEU
MET MET
GLN GLN
TYR TYR
HIS HIS
VAL VAL
PHE PHE
VAL VAL
MET MET
THR THR
PHE PHE
LEU LEU
CYS CYS
THR THR
ILE ILE
LEU LEU
SER SER
ASP ASP
ALA ALA
TYR TYR
ASN ASN
PHE PHE

GLY VAL
LEU LEU
GLU GLU
ALA ALA
TYR TYR
LEU LEU
MET MET
ASP ASP
SER SER
GLN GLN
ASP ASP
PHE PHE
GLN GLN
ILE ILE
PRO PRO
VAL VAL
SER SER
GLU GLU
VAL VAL
MET MET
ASN ASN
ASP ASP
ASP ASP
LEU LEU
GLN GLN
LYS LYS
SER SER
VAL VAL
ASP ASP
MET MET
ILE ILE
MET MET
SER SER
SER SER
MET MET
PHE PHE
CYS CYS
PRO PRO
PRO PRO
GLY GLY
ILE ILE
LYS LYS
ILE ILE
ASP ASP
ALA ALA
TYR TYR
PRO PRO
TRP TRP
LEU LEU
GLU GLU
CYS CYS
PHE PHE
ILE ILE
LYS LYS
SER SER
TYR TYR
ASN ASN
VAL VAL

THR
ASN
GLY
THR
ASP
ASN
GLN
ILE
CYS
TYR
GLN
ILE
PHE
ASP
THR
THR
VAL
ALA
GLU
ASP
VAL
VAL
ILE

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	192871	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	45871	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	305.2, 305.2, 305.2	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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	0.66	5/7810 (0.1%)	0.81	1/10584 (0.0%)
2	B	0.41	0/6055	0.91	14/9426 (0.1%)
3	L	0.52	0/650	0.71	0/874
4	M	0.50	0/710	0.60	0/957
5	N	0.41	0/517	0.89	0/798
6	O	0.34	0/968	0.63	1/1307 (0.1%)
7	P	0.36	0/2048	0.57	2/2774 (0.1%)
All	All	0.53	5/18758 (0.0%)	0.81	18/26720 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
5	N	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	638	TYR	CE1-CZ	10.15	1.51	1.38
1	A	638	TYR	CG-CD1	7.25	1.48	1.39
1	A	638	TYR	CG-CD2	7.20	1.48	1.39
1	A	638	TYR	CE2-CZ	7.02	1.47	1.38
1	A	547	TRP	CD2-CE2	5.52	1.48	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	142	C	C2'-C3'-O3'	8.95	129.19	109.50
7	P	188	ARG	NE-CZ-NH2	8.30	124.45	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	188	ARG	NE-CZ-NH1	-7.73	116.44	120.30
2	B	131	C	C5'-C4'-O4'	7.07	117.58	109.10
2	B	174	A	C2'-C3'-O3'	6.97	124.85	113.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	75	C	Sidechain
5	N	27	DA	Sidechain

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	7626	0	7871	131	0
2	B	5431	0	2767	65	0
3	L	643	0	680	8	0
4	M	699	0	712	5	0
5	N	461	0	253	2	0
6	O	955	0	962	13	0
7	P	2005	0	2033	21	0
All	All	17820	0	15278	213	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 6.

The worst 5 of 213 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)
7:P:184:TRP:CZ3	7:P:292:LEU:HD22	1.85	1.10
1:A:1072:TRP:HE1	1:A:1104:SER:HG	1.07	0.97
6:O:192:GLN:HB2	6:O:203:TYR:CD2	2.06	0.89
7:P:184:TRP:CE3	7:P:292:LEU:HD22	2.08	0.88
2:B:302:A:N7	4:M:57:SER:HB2	1.94	0.82

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	943/1132 (83%)	876 (93%)	61 (6%)	6 (1%)	25	63
3	L	80/130 (62%)	79 (99%)	1 (1%)	0	100	100
4	M	88/166 (53%)	83 (94%)	5 (6%)	0	100	100
6	O	112/458 (24%)	110 (98%)	2 (2%)	0	100	100
7	P	243/634 (38%)	236 (97%)	7 (3%)	0	100	100
All	All	1466/2520 (58%)	1384 (94%)	76 (5%)	6 (0%)	38	71

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	982	CYS
1	A	164	PRO
1	A	1087	VAL
1	A	643	ARG
1	A	570	LYS

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	824/958 (86%)	816 (99%)	8 (1%)	76	86
3	L	64/99 (65%)	64 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	M	77/140 (55%)	77 (100%)	0	100	100
6	O	106/390 (27%)	106 (100%)	0	100	100
7	P	226/576 (39%)	226 (100%)	0	100	100
All	All	1297/2163 (60%)	1289 (99%)	8 (1%)	86	91

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1129	THR
1	A	1074	CYS
1	A	962	ARG
1	A	558	ARG
1	A	970	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1013	HIS
4	M	64	ASN
7	P	264	HIS
7	P	24	ASN
7	P	160	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	252/451 (55%)	74 (29%)	21 (8%)

5 of 74 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	27	G
2	B	28	G
2	B	29	U
2	B	30	G
2	B	37	A

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	262	C
2	B	300	G
2	B	321	C
2	B	307	U
2	B	292	G

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](#)

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.

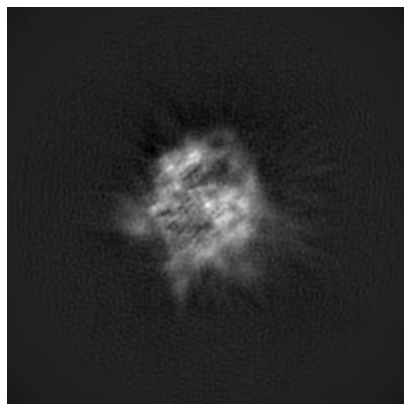
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14197. These allow visual inspection of the internal detail of the map and identification of artifacts.

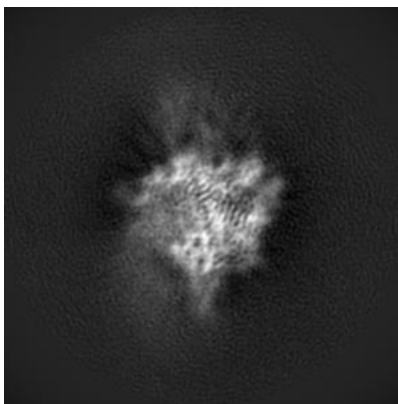
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

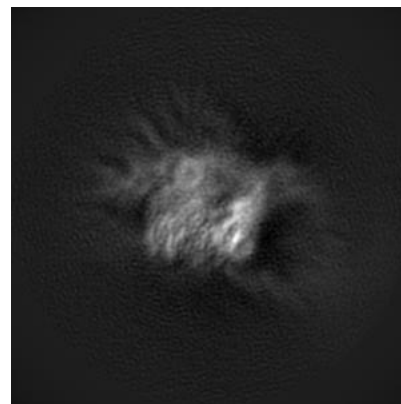
6.1.1 Primary map



X

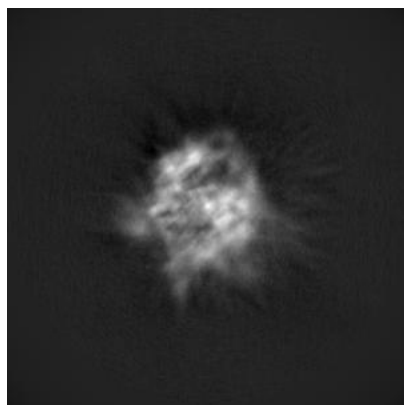


Y

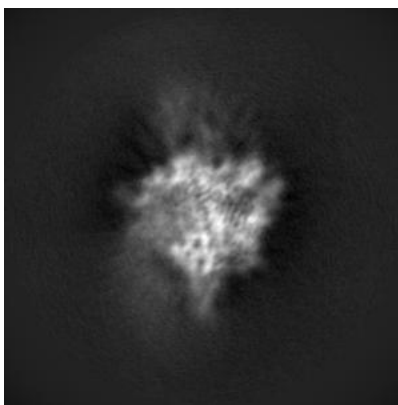


Z

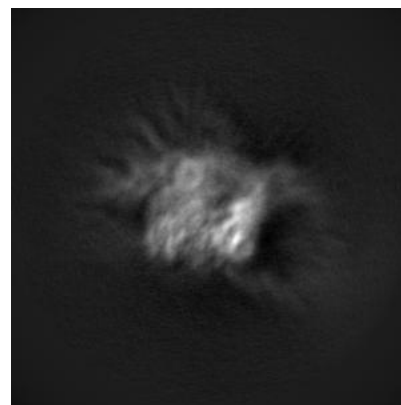
6.1.2 Raw map



X



Y

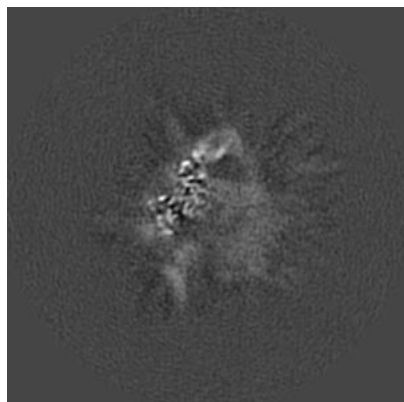


Z

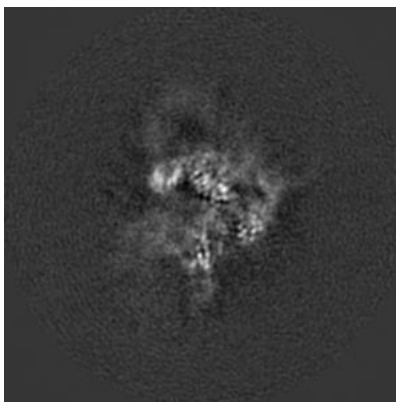
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

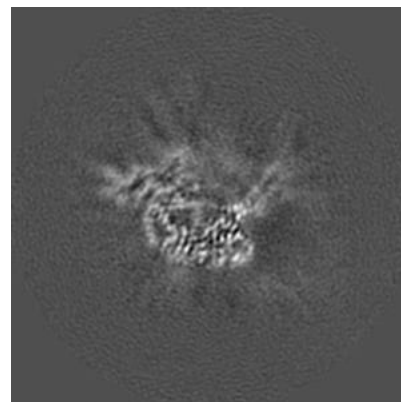
6.2.1 Primary map



X Index: 140

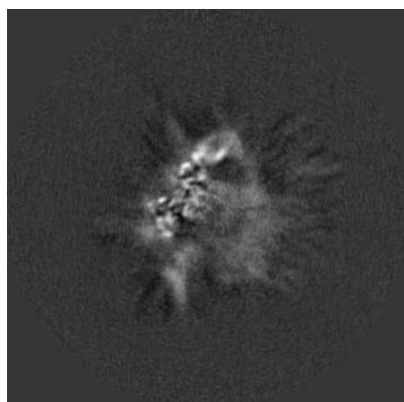


Y Index: 140

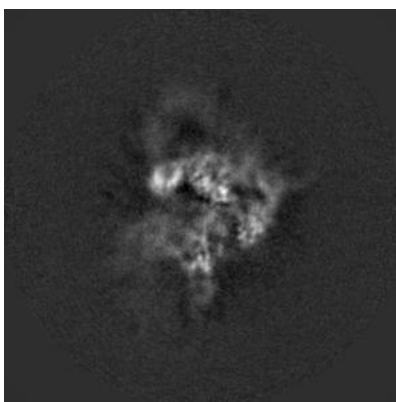


Z Index: 140

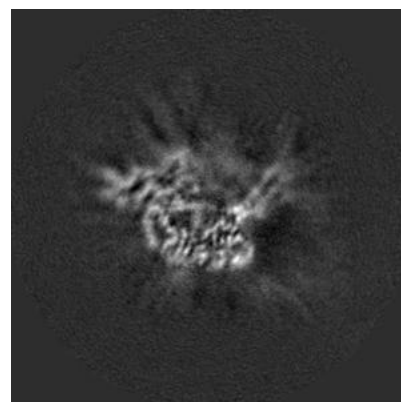
6.2.2 Raw map



X Index: 140



Y Index: 140

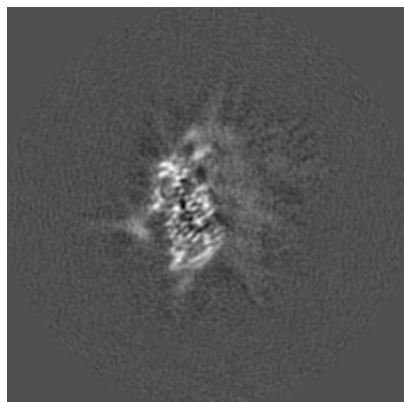


Z Index: 140

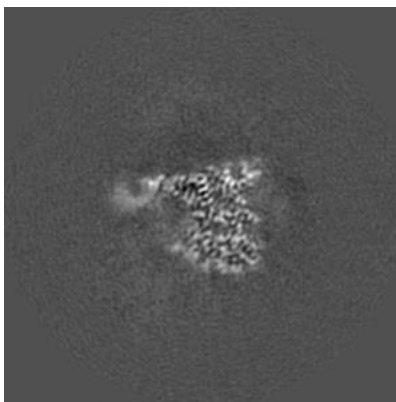
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

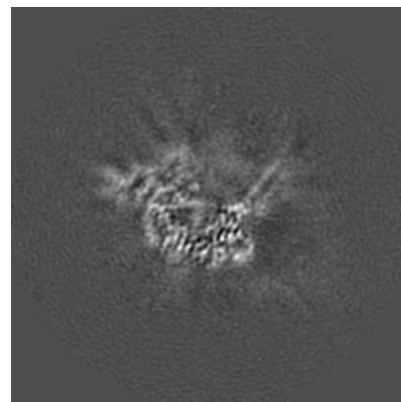
6.3.1 Primary map



X Index: 157

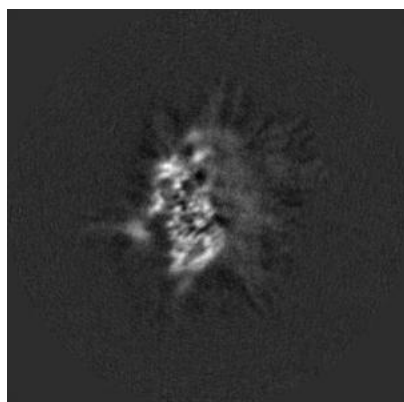


Y Index: 119

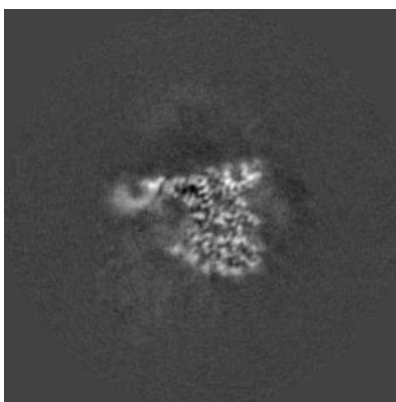


Z Index: 141

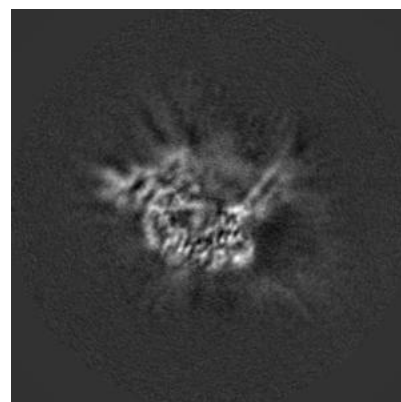
6.3.2 Raw map



X Index: 158



Y Index: 119

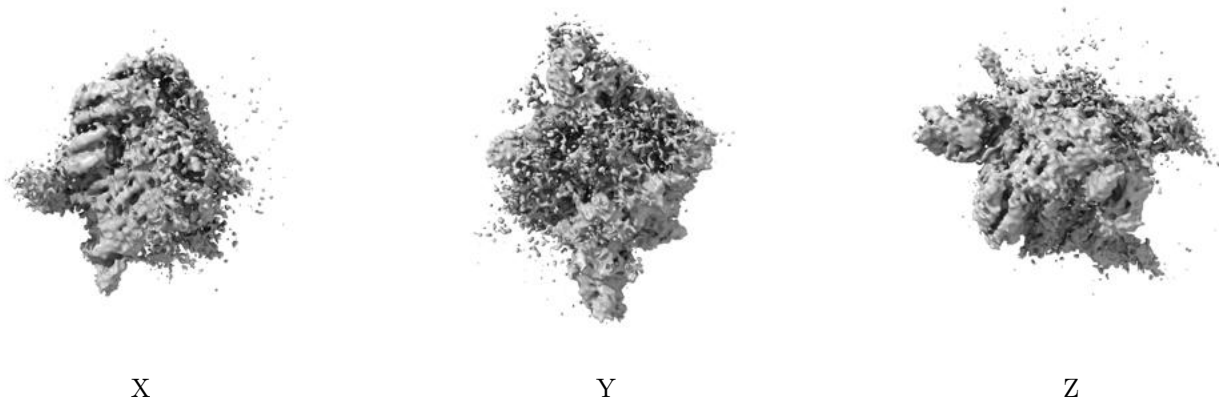


Z Index: 141

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

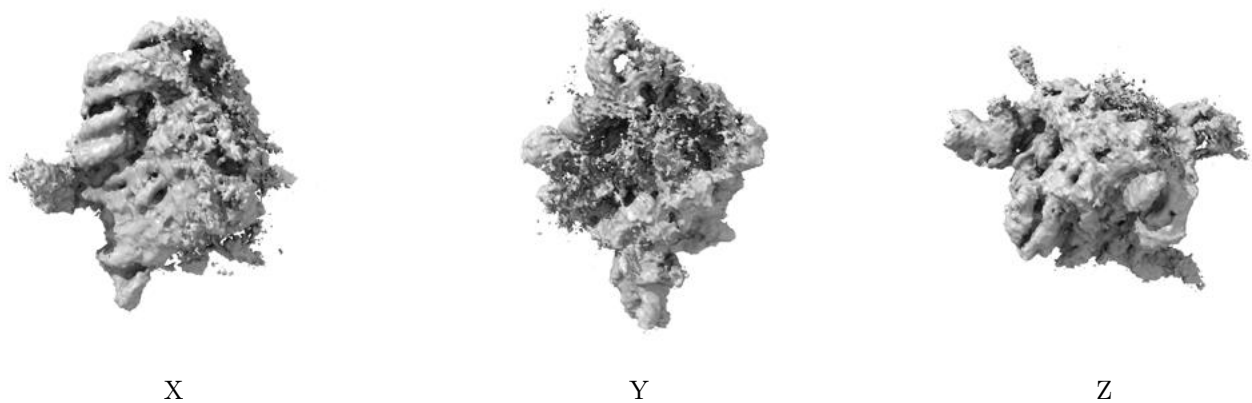
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

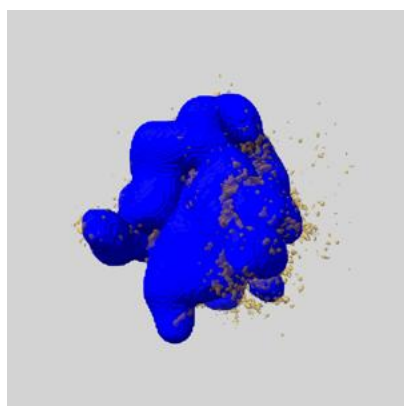
6.5 Mask visualisation [i](#)

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

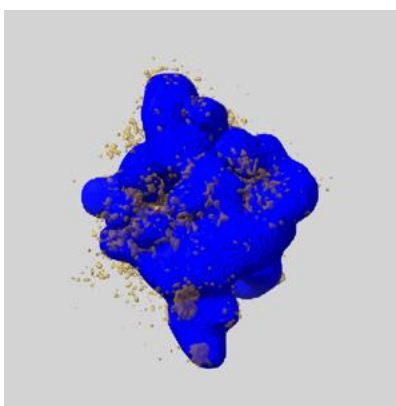
A mask typically either:

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

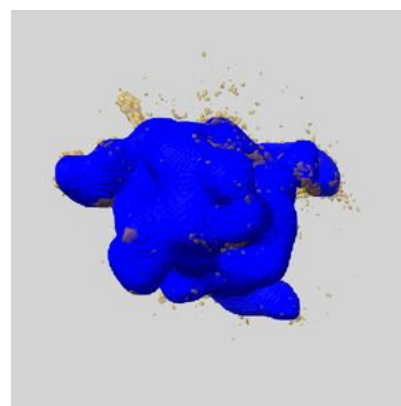
6.5.1 emd_14197_msk_1.map [i](#)



X



Y

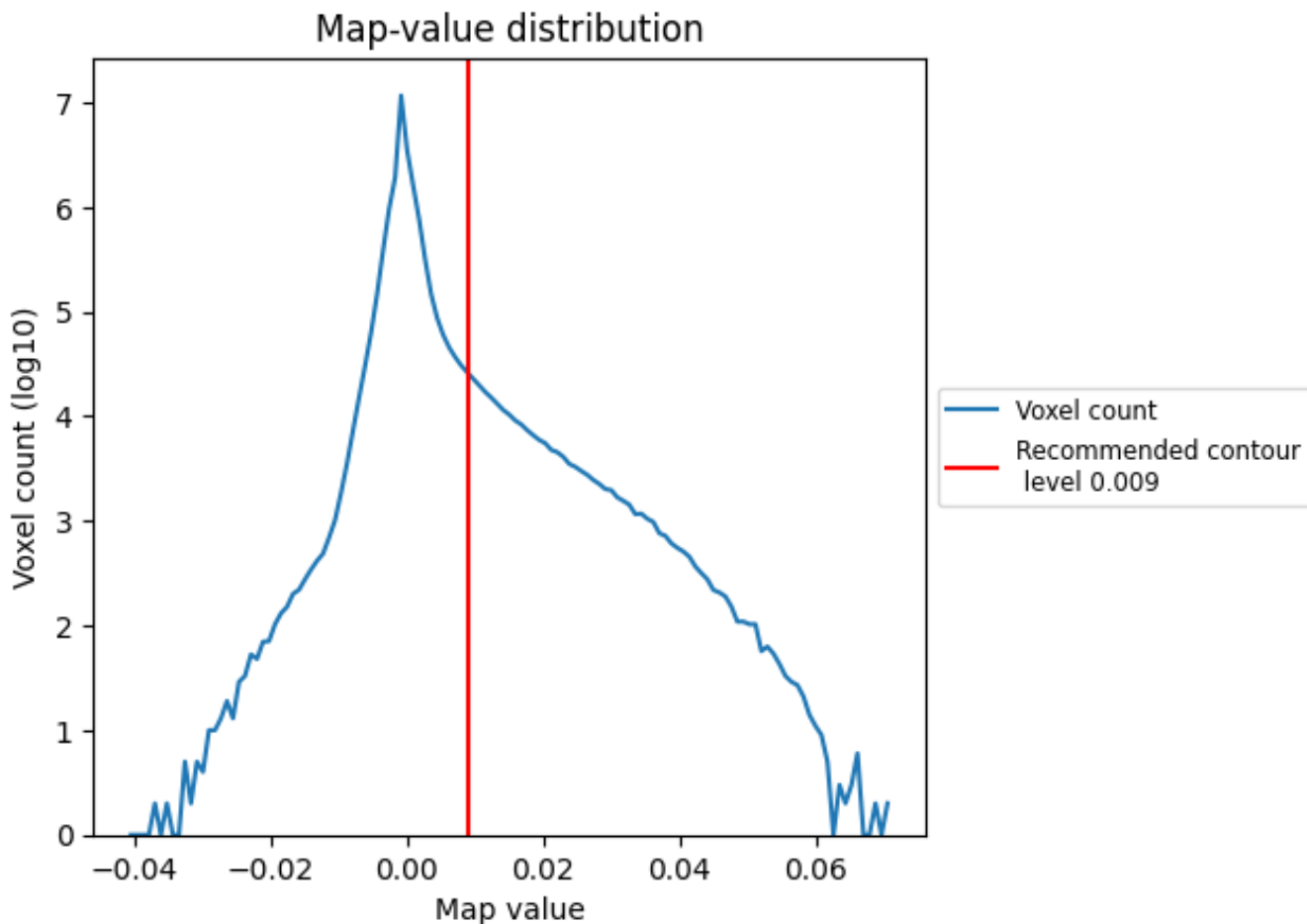


Z

7 Map analysis [i](#)

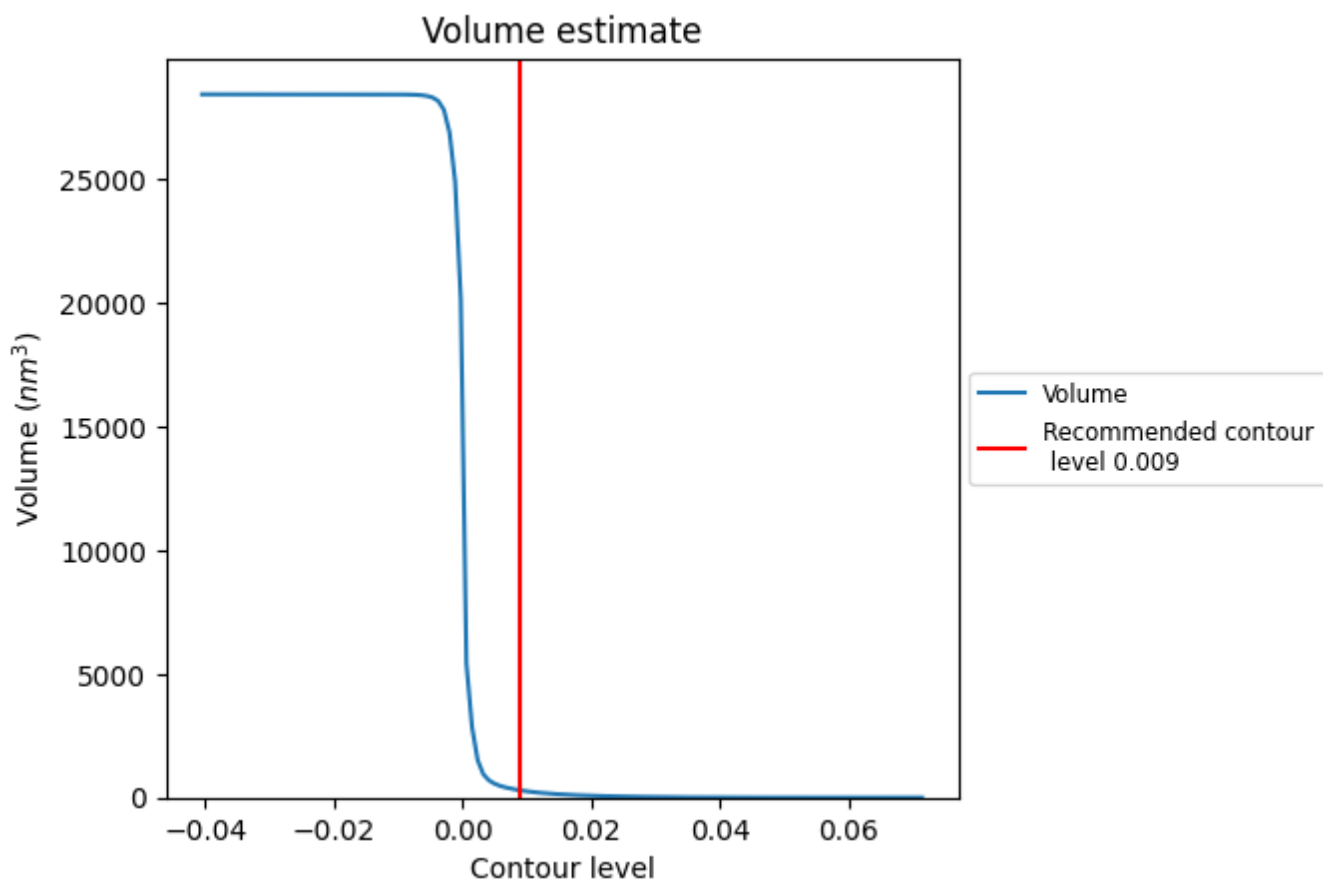
This section contains the results of statistical analysis of the map.

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.

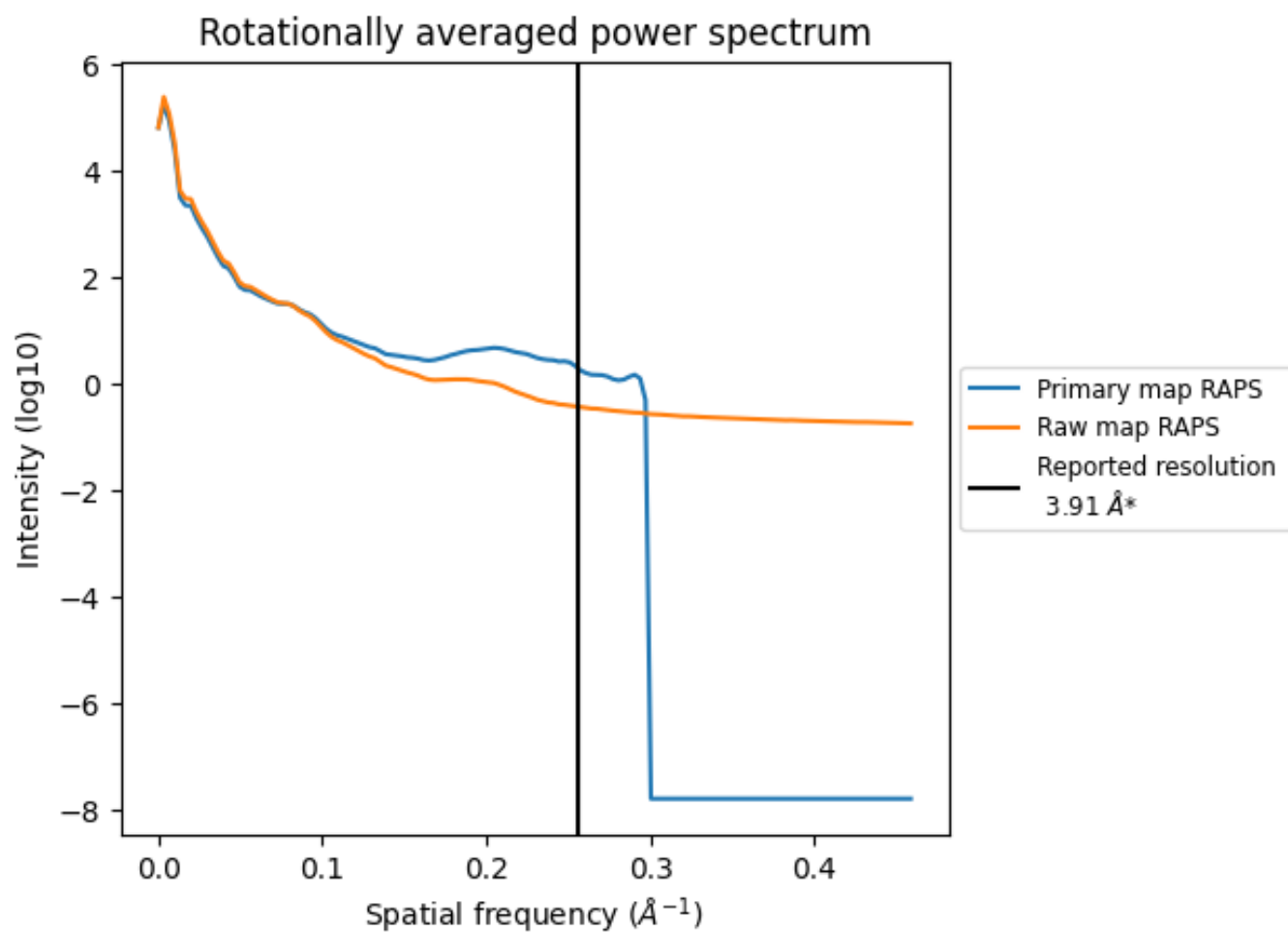
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 291 nm³; this corresponds to an approximate mass of 263 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

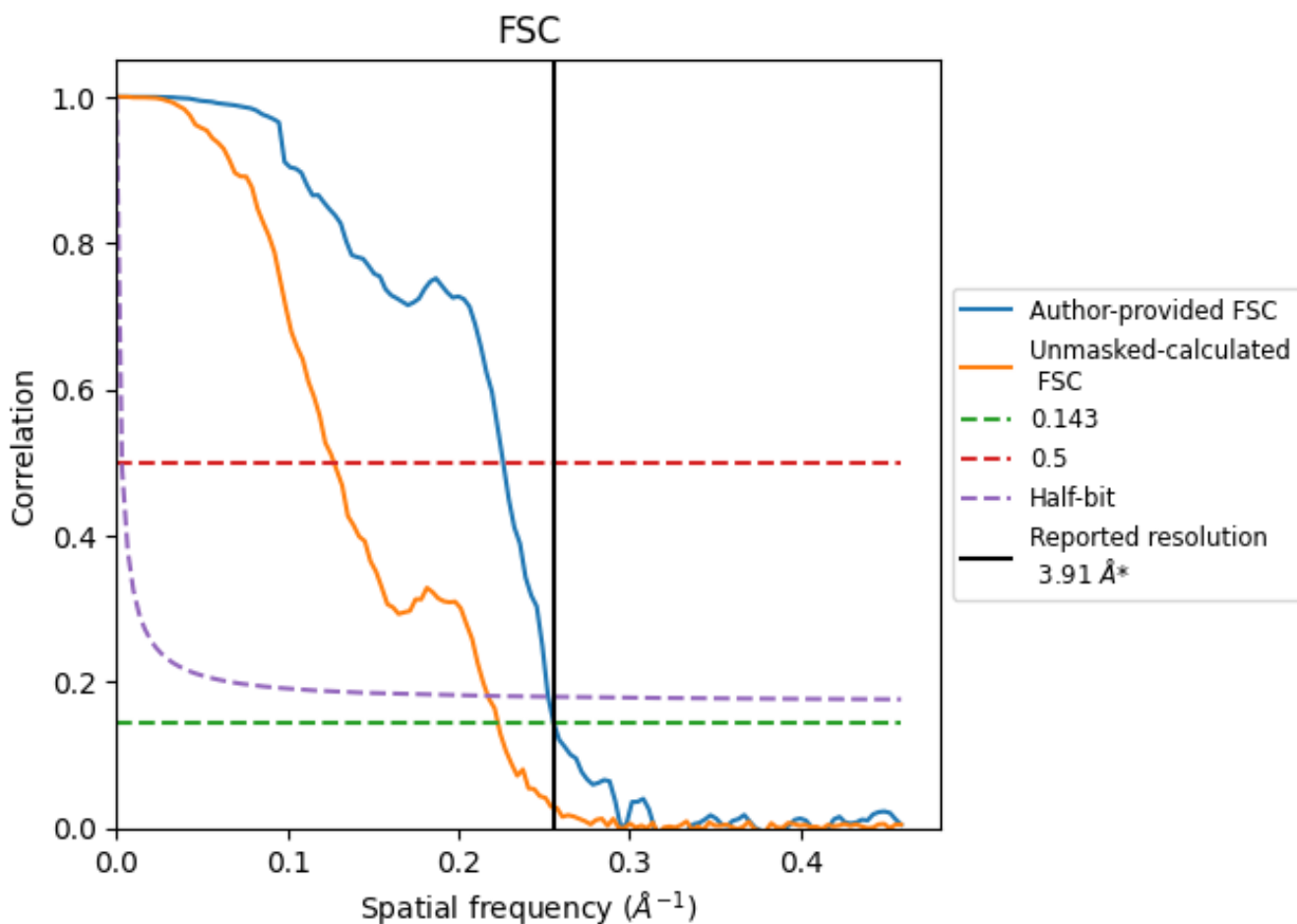


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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](#)

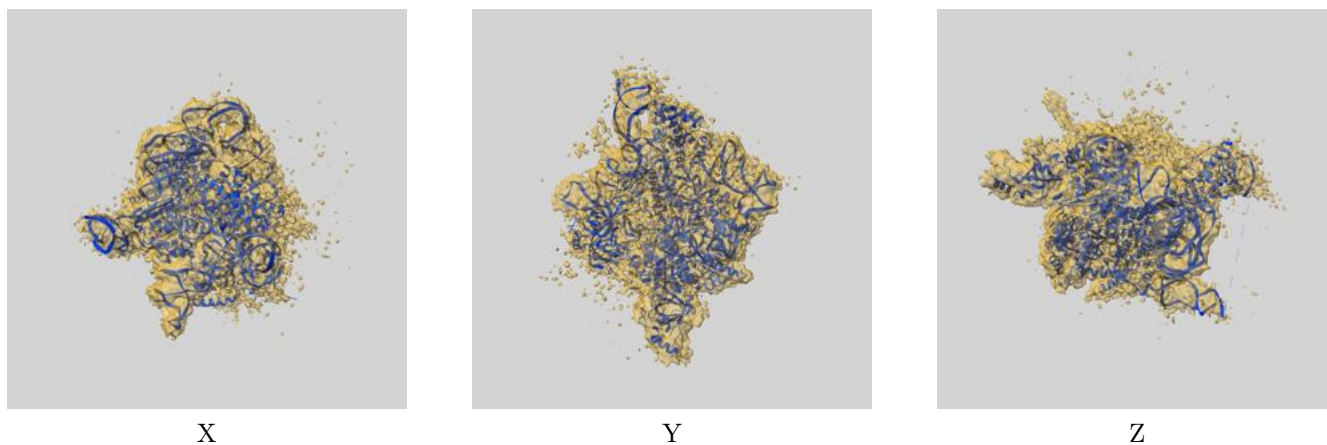
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.91	-	-
Author-provided FSC curve	3.91	4.42	3.96
Unmasked-calculated*	4.48	7.87	4.60

*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 4.48 differs from the reported value 3.91 by more than 10 %

9 Map-model fit [i](#)

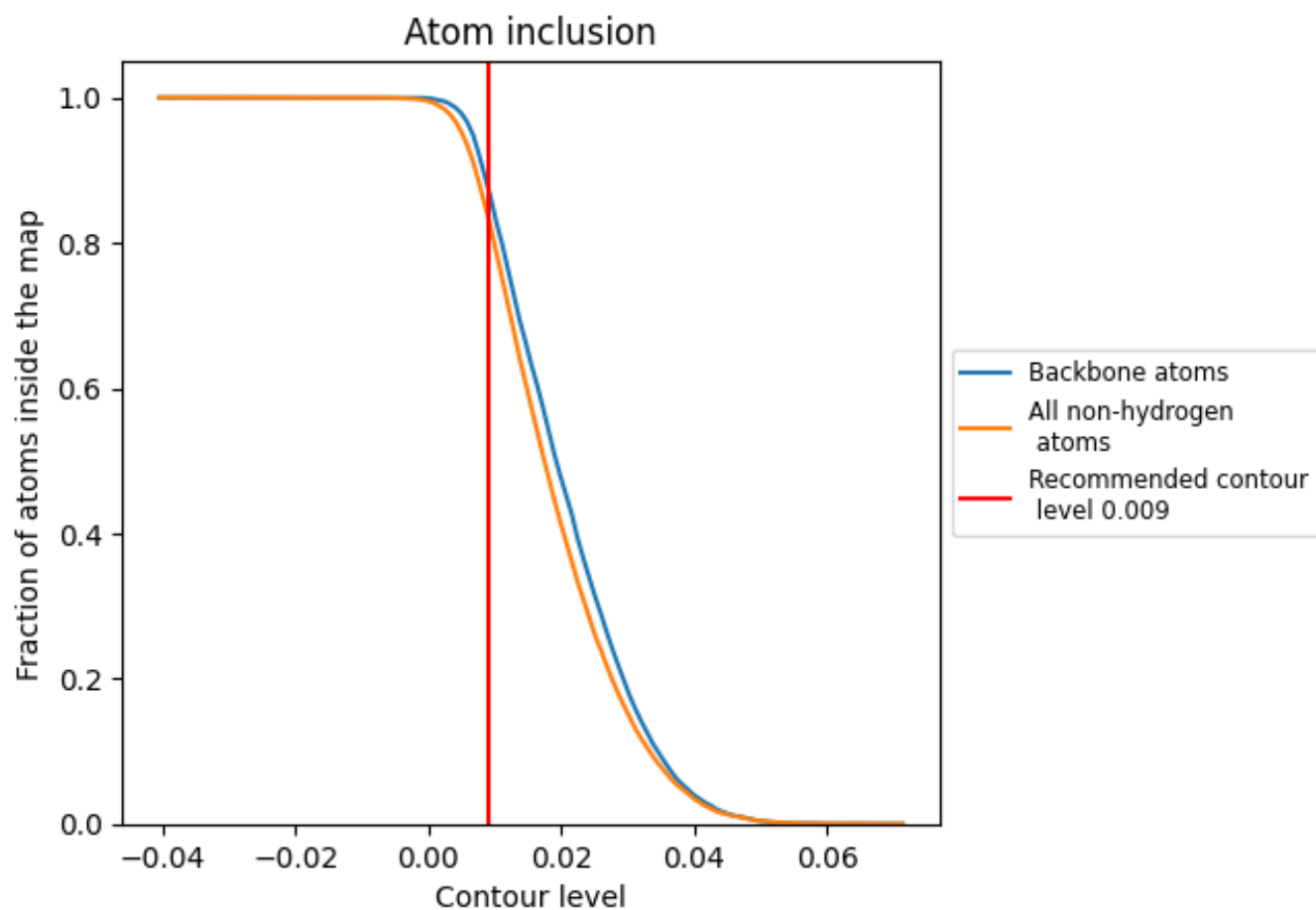
This section contains information regarding the fit between EMDB map EMD-14197 and PDB model 7QXS. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.009 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, 88% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.