



wwPDB EM Map/Model Validation Summary Report ⓘ

Aug 29, 2020 – 05:50 PM BST

PDB ID : 6N7R
EMDB ID : EMD-0361
Title : Saccharomyces cerevisiae spliceosomal E complex (ACT1)
Authors : Liu, S.; Li, X.; Zhou, Z.H.; Zhao, R.
Deposited on : 2018-11-28
Resolution : 3.20 Å(reported)

This is a wwPDB EM Map/Model 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:

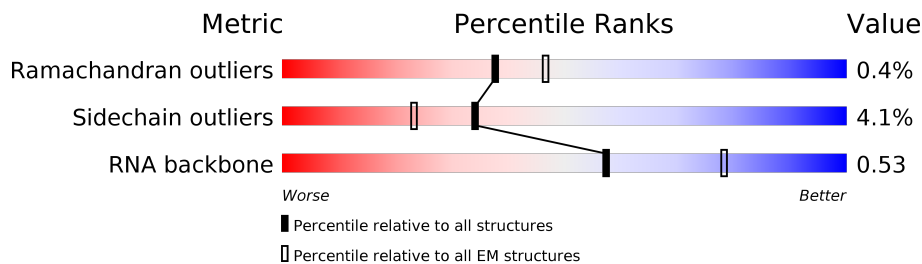
EMDB validation analysis : 0.0.0.dev33
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

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 3.20 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)
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 on 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	300	
2	B	231	
3	C	350	
4	D	544	
5	E	629	
6	F	523	
7	G	492	
8	H	89	

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Mol	Chain	Length	Quality of chain
9	I	261	
10	K	196	
11	L	146	
12	M	110	
13	N	101	
14	O	94	
15	P	86	
16	Q	77	
17	R	568	
18	r	240	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 35750 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 U1 small nuclear ribonucleoprotein 70 kDa homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	186	1217	751	229	235	2	0	0

- Molecule 2 is a protein called U1 small nuclear ribonucleoprotein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	195	1567	974	301	286	6	0	0

- Molecule 3 is a protein called U1 small nuclear ribonucleoprotein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	133	1053	669	192	188	4	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	299	GLY	-	expression tag	UNP P32605
C	300	ARG	-	expression tag	UNP P32605
C	301	ARG	-	expression tag	UNP P32605
C	302	ILE	-	expression tag	UNP P32605
C	303	PRO	-	expression tag	UNP P32605
C	304	GLY	-	expression tag	UNP P32605
C	305	LEU	-	expression tag	UNP P32605
C	306	ILE	-	expression tag	UNP P32605
C	307	ASN	-	expression tag	UNP P32605
C	308	PRO	-	expression tag	UNP P32605
C	309	TRP	-	expression tag	UNP P32605
C	310	LYS	-	expression tag	UNP P32605
C	311	ARG	-	expression tag	UNP P32605
C	312	ARG	-	expression tag	UNP P32605
C	313	TRP	-	expression tag	UNP P32605

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Chain	Residue	Modelled	Actual	Comment	Reference
C	314	LYS	-	expression tag	UNP P32605
C	315	LYS	-	expression tag	UNP P32605
C	316	ASN	-	expression tag	UNP P32605
C	317	PHE	-	expression tag	UNP P32605
C	318	ILE	-	expression tag	UNP P32605
C	319	ALA	-	expression tag	UNP P32605
C	320	VAL	-	expression tag	UNP P32605
C	321	SER	-	expression tag	UNP P32605
C	322	ALA	-	expression tag	UNP P32605
C	323	ALA	-	expression tag	UNP P32605
C	324	ASN	-	expression tag	UNP P32605
C	325	ARG	-	expression tag	UNP P32605
C	326	PHE	-	expression tag	UNP P32605
C	327	LYS	-	expression tag	UNP P32605
C	328	LYS	-	expression tag	UNP P32605
C	329	ILE	-	expression tag	UNP P32605
C	330	SER	-	expression tag	UNP P32605
C	331	SER	-	expression tag	UNP P32605
C	332	SER	-	expression tag	UNP P32605
C	333	GLY	-	expression tag	UNP P32605
C	334	ALA	-	expression tag	UNP P32605
C	335	LEU	-	expression tag	UNP P32605
C	336	ASP	-	expression tag	UNP P32605
C	337	TYR	-	expression tag	UNP P32605
C	338	ASP	-	expression tag	UNP P32605
C	339	ILE	-	expression tag	UNP P32605
C	340	PRO	-	expression tag	UNP P32605
C	341	THR	-	expression tag	UNP P32605
C	342	THR	-	expression tag	UNP P32605
C	343	ALA	-	expression tag	UNP P32605
C	344	SER	-	expression tag	UNP P32605
C	345	GLU	-	expression tag	UNP P32605
C	346	ASN	-	expression tag	UNP P32605
C	347	LEU	-	expression tag	UNP P32605
C	348	TYR	-	expression tag	UNP P32605
C	349	PHE	-	expression tag	UNP P32605
C	350	GLN	-	expression tag	UNP P32605

- Molecule 4 is a protein called U1 small nuclear ribonucleoprotein component PRP42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	541	4523	2968	719	816	20	0	0

- Molecule 5 is a protein called Pre-mRNA-processing factor 39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	576	3985	2530	694	752	9	0	0

- Molecule 6 is a protein called Protein NAM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	185	1416	889	243	273	11	0	0

- Molecule 7 is a protein called 56 kDa U1 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	232	1897	1232	310	343	12	0	0

- Molecule 8 is a protein called U1 small nuclear ribonucleoprotein component SNU71,U1 small nuclear ribonucleoprotein component SNU71,Snu71.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	89	605	377	111	116	1	0	0

- Molecule 9 is a protein called Protein LUC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	147	1166	731	211	213	11	0	0

- Molecule 10 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	124	1012	638	192	179	3	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	119	921	578	164	176	3	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	107	862	547	159	152	4	0	0

- Molecule 13 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	91	695	443	119	130	3	0	0

- Molecule 14 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	75	573	381	92	97	3	0	0

- Molecule 15 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	74	580	375	103	101	1	0	0

- Molecule 16 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	71	537	342	95	99	1	0	0

- Molecule 17 is a RNA chain called U1 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	R	558	11817	5287	2003	3970	557	0	0

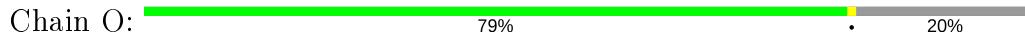
- Molecule 18 is a RNA chain called ACT1 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	r	63	1323	597	217	446	63	0	0

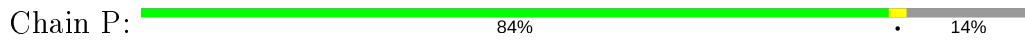
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total 1	Zn 1	0

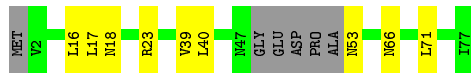
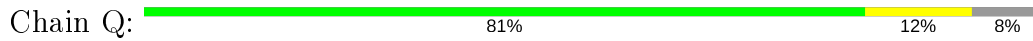
• Molecule 14: Small nuclear ribonucleoprotein E



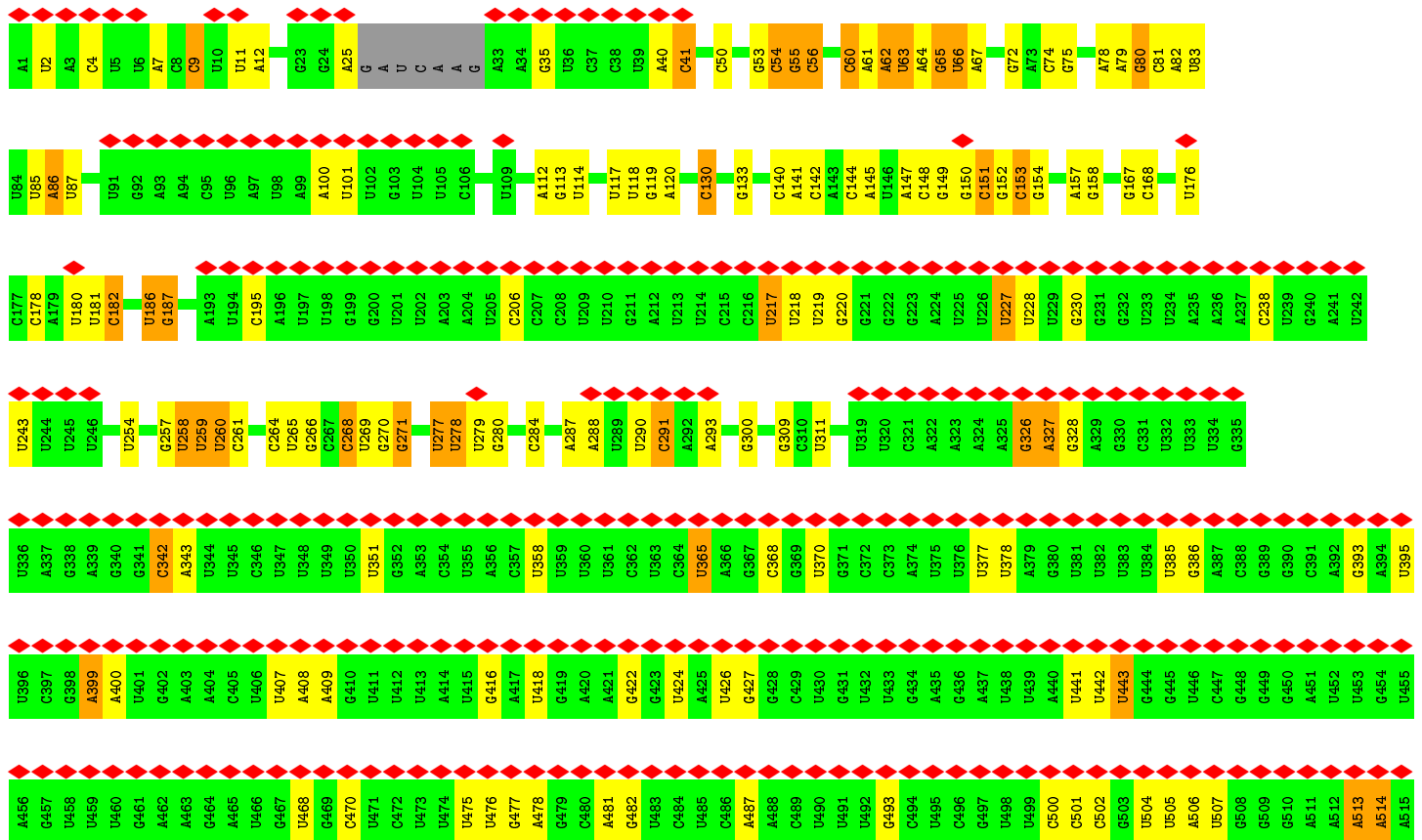
• Molecule 15: Small nuclear ribonucleoprotein F



• Molecule 16: Small nuclear ribonucleoprotein G



• Molecule 17: U1 snRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	270587	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 ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.312	Depositor
Minimum map value	-0.152	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	478.72, 478.72, 478.72	Depositor
Map dimensions	352, 352, 352	Depositor
Map angles (°)	90.0, 90.0, 90.0	Depositor
Pixel spacing (Å)	1.36, 1.36, 1.36	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:
ZN

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	0.70	0/1235	0.67	2/1689 (0.1%)
2	B	0.85	0/1598	0.80	4/2150 (0.2%)
3	C	0.53	0/1066	0.74	0/1430
4	D	1.13	2/4637 (0.0%)	0.86	10/6270 (0.2%)
5	E	0.78	1/4050 (0.0%)	0.67	1/5543 (0.0%)
6	F	1.02	1/1443 (0.1%)	0.80	1/1957 (0.1%)
7	G	0.91	1/1938 (0.1%)	0.81	2/2605 (0.1%)
8	H	0.79	1/428 (0.2%)	0.67	0/575
9	I	0.42	0/1186	0.64	0/1594
10	K	0.94	0/1018	0.87	0/1355
11	L	0.87	0/930	0.90	0/1261
12	M	0.79	0/876	0.75	1/1179 (0.1%)
13	N	1.08	1/707 (0.1%)	0.80	0/959
14	O	0.88	0/583	0.80	0/791
15	P	0.96	0/593	0.85	0/804
16	Q	0.91	0/540	0.85	1/727 (0.1%)
17	R	1.05	17/13195 (0.1%)	1.28	142/20542 (0.7%)
18	r	0.55	0/234	1.12	0/362
All	All	0.95	24/36257 (0.1%)	1.01	164/51793 (0.3%)

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	R	72	G	N7-C5	-5.99	1.35	1.39
6	F	356	VAL	CB-CG1	-5.97	1.40	1.52
17	R	559	G	N9-C8	-5.89	1.33	1.37
17	R	564	A	N7-C5	-5.84	1.35	1.39
17	R	559	G	N7-C5	-5.77	1.35	1.39

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	227	U	N1-C2-O2	12.11	131.28	122.80
17	R	227	U	C2-N1-C1'	11.75	131.80	117.70
17	R	151	C	N3-C2-O2	-11.59	113.79	121.90
17	R	227	U	N3-C2-O2	-11.37	114.24	122.20
17	R	442	U	OP2-P-O3'	-11.06	80.86	105.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	182/300 (61%)	166 (91%)	14 (8%)	2 (1%)	14	51
2	B	193/231 (84%)	179 (93%)	14 (7%)	0	100	100
3	C	127/350 (36%)	122 (96%)	4 (3%)	1 (1%)	19	58
4	D	539/544 (99%)	515 (96%)	23 (4%)	1 (0%)	47	79
5	E	570/629 (91%)	546 (96%)	24 (4%)	0	100	100
6	F	179/523 (34%)	166 (93%)	12 (7%)	1 (1%)	25	64
7	G	226/492 (46%)	211 (93%)	13 (6%)	2 (1%)	17	56
8	H	50/89 (56%)	50 (100%)	0	0	100	100
9	I	141/261 (54%)	134 (95%)	6 (4%)	1 (1%)	22	61
10	K	120/196 (61%)	116 (97%)	4 (3%)	0	100	100
11	L	117/146 (80%)	105 (90%)	10 (8%)	2 (2%)	9	42
12	M	105/110 (96%)	103 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	N	89/101 (88%)	85 (96%)	4 (4%)	0	100	100
14	O	71/94 (76%)	69 (97%)	2 (3%)	0	100	100
15	P	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
16	Q	67/77 (87%)	64 (96%)	3 (4%)	0	100	100
All	All	2848/4229 (67%)	2700 (95%)	138 (5%)	10 (0%)	38	69

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	PRO
7	G	208	VAL
4	D	43	PRO
6	F	411	GLN
1	A	37	THR

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	84/265 (32%)	81 (96%)	3 (4%)	35	69
2	B	171/214 (80%)	167 (98%)	4 (2%)	50	78
3	C	116/317 (37%)	108 (93%)	8 (7%)	15	49
4	D	502/519 (97%)	486 (97%)	16 (3%)	39	71
5	E	317/603 (53%)	306 (96%)	11 (4%)	36	69
6	F	157/451 (35%)	151 (96%)	6 (4%)	33	67
7	G	212/448 (47%)	196 (92%)	16 (8%)	13	45
8	H	48/48 (100%)	48 (100%)	0	100	100
9	I	123/234 (53%)	116 (94%)	7 (6%)	20	56
10	K	114/176 (65%)	110 (96%)	4 (4%)	36	69
11	L	107/129 (83%)	102 (95%)	5 (5%)	26	62
12	M	96/103 (93%)	94 (98%)	2 (2%)	53	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	N	79/89 (89%)	77 (98%)	2 (2%)	47 77
14	O	63/83 (76%)	62 (98%)	1 (2%)	62 84
15	P	63/77 (82%)	61 (97%)	2 (3%)	39 71
16	Q	57/66 (86%)	49 (86%)	8 (14%)	3 16
All	All	2309/3822 (60%)	2214 (96%)	95 (4%)	34 66

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	317	ILE
7	G	98	LEU
16	Q	16	LEU
6	F	340	VAL
7	G	89	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	412	GLN
9	I	40	HIS
15	P	65	HIS
6	F	432	ASN
6	F	442	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	R	555/568 (97%)	126 (22%)	19 (3%)
18	r	9/240 (3%)	1 (11%)	0
All	All	564/808 (69%)	127 (22%)	19 (3%)

5 of 127 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	R	7	A
17	R	9	C
17	R	11	U
17	R	12	A
17	R	35	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	R	152	G
17	R	258	U
17	R	342	C
17	R	151	C
17	R	399	A

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	r	2
8	H	1

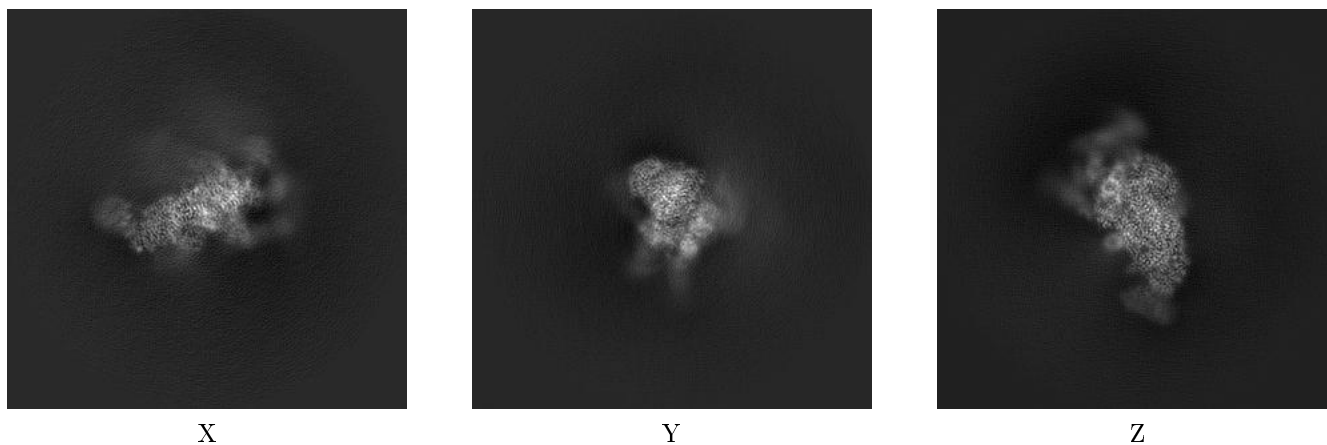
All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	52:SER	C	1262:UNK	N	67.13
1	r	8:C	O3'	103:N	P	54.79
1	r	128:N	O3'	130:N	P	17.87

6 Map visualisation [i](#)

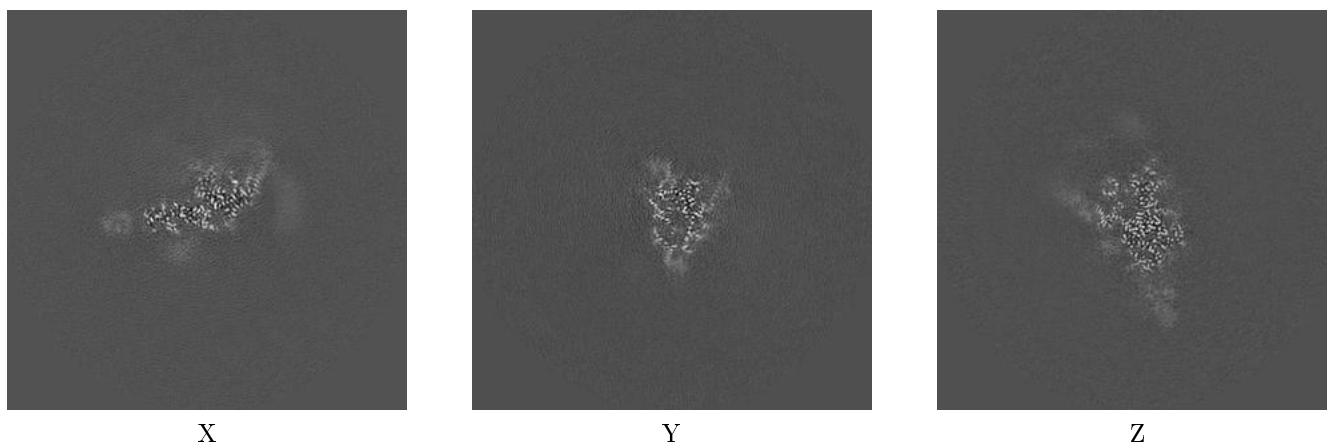
This section contains visualisations of the EMDB entry EMD-0361. These are intended to permit visual inspection of the internal detail of the map and identification of artifacts.

6.1 Orthogonal projections [i](#)



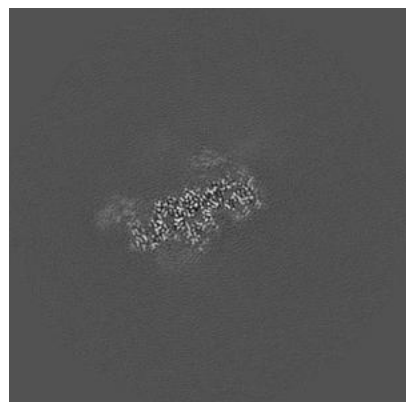
The images above show the map projected in three orthogonal projections, in greyscale.

6.2 Central slices [i](#)

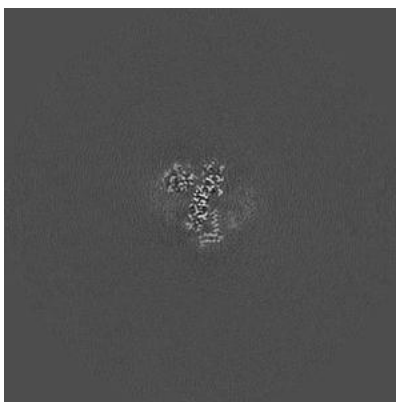


The images above show central slices of the map in three orthogonal directions, in greyscale.

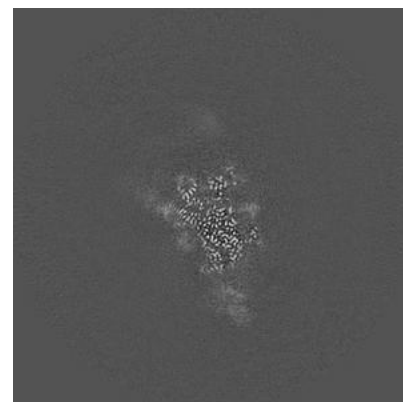
6.3 Largest variance slices [i](#)



X Index: 191



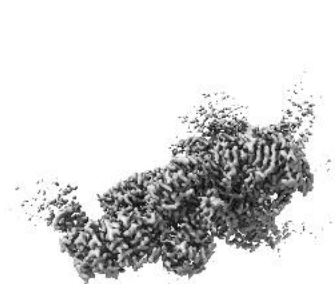
Y Index: 161



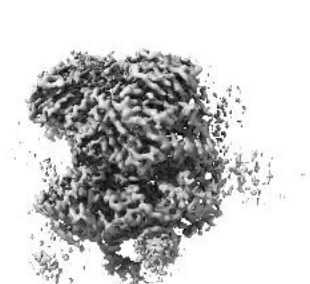
Z Index: 173

The images above show the highest variance slices of the map in three orthogonal directions, in greyscale.

6.4 Orthogonal surface views [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. This in conjunction with the slice images can indicate whether an appropriate contour level has been selected.

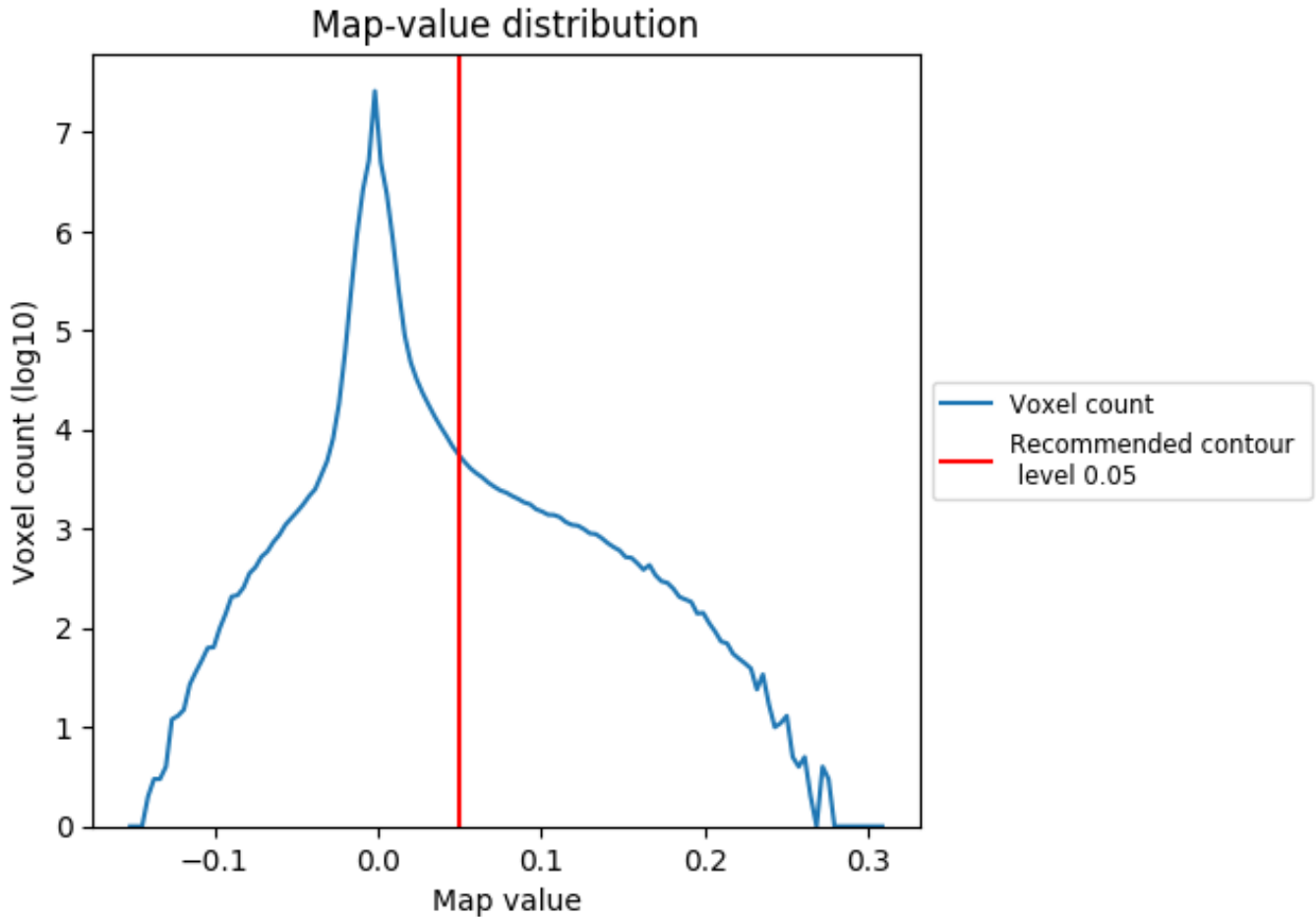
6.5 Mask visualisation [i](#)

This section was not generated. No masks were provided.

7 Map analysis [i](#)

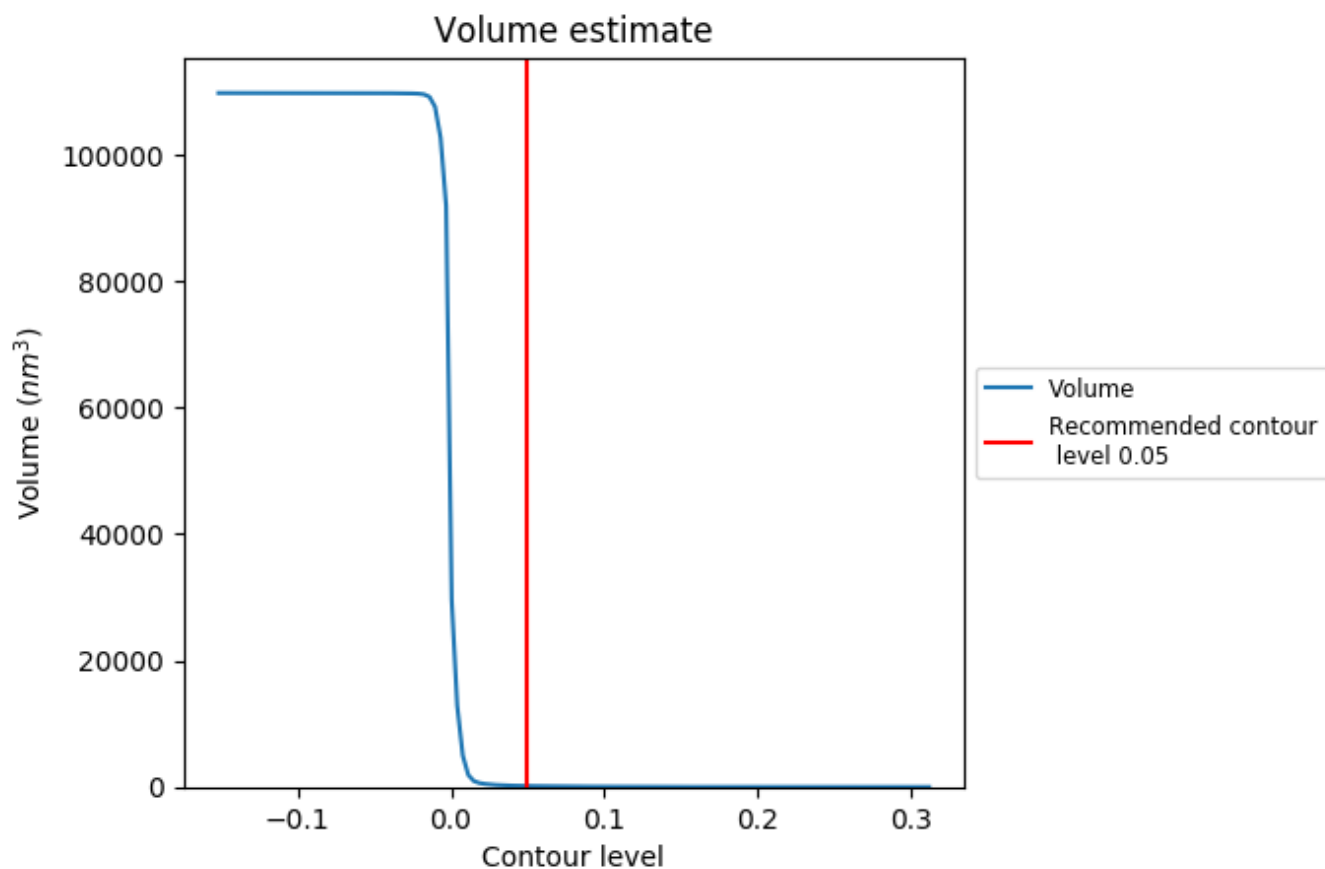
This section contains the results of statistical analysis of the map.

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.

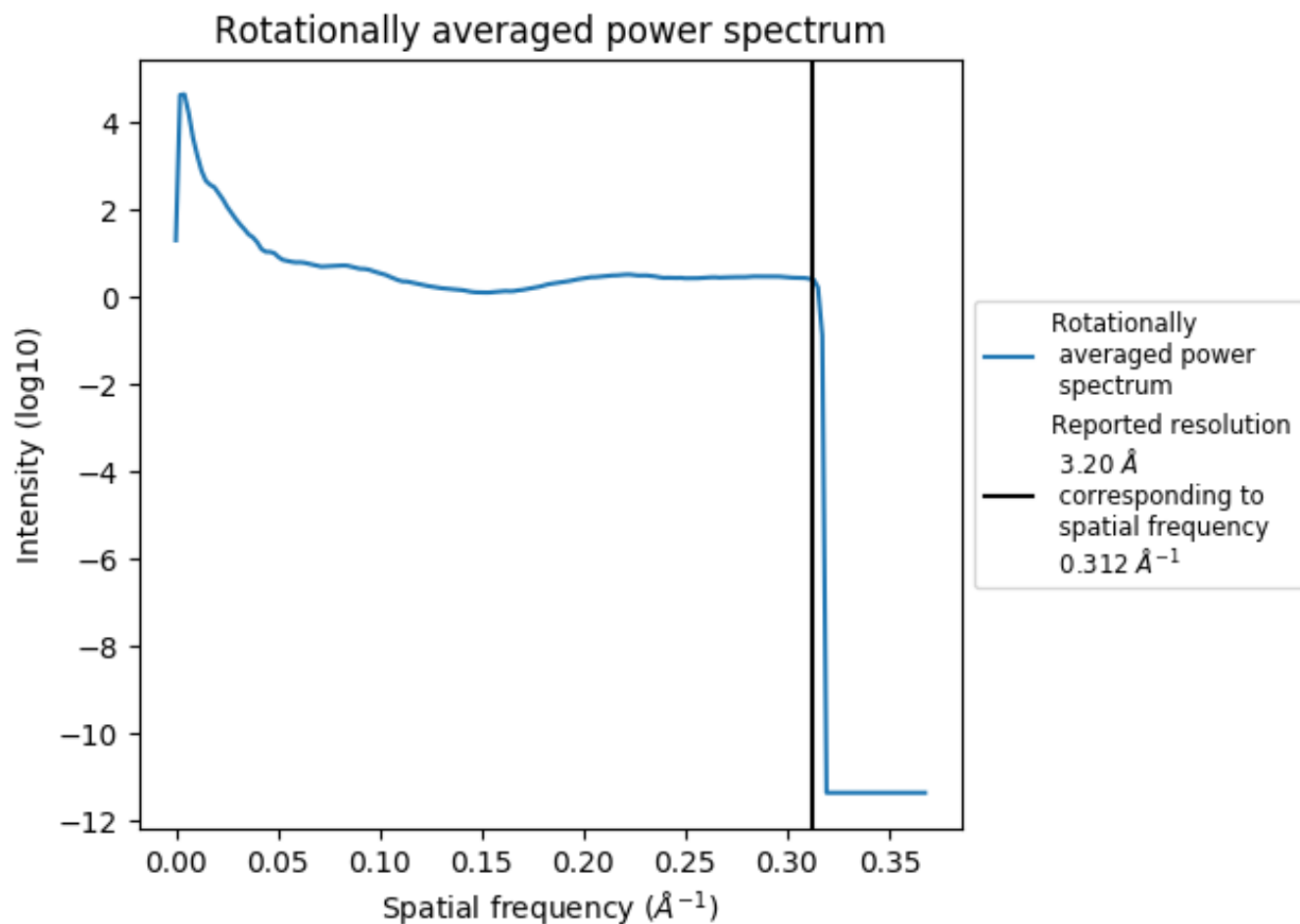
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm^3 ; this corresponds to an approximate mass of 135 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 [\(i\)](#)



8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution for single-particle and subtomogram-averaging methods. 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. Curves are displayed for 3σ , 1-bit and 1/2-bit in addition to lines showing the 0.143 gold standard cut-off, 0.333 cut-off and legacy 0.5 cut-off.

8.1 Resolution estimates [i](#)

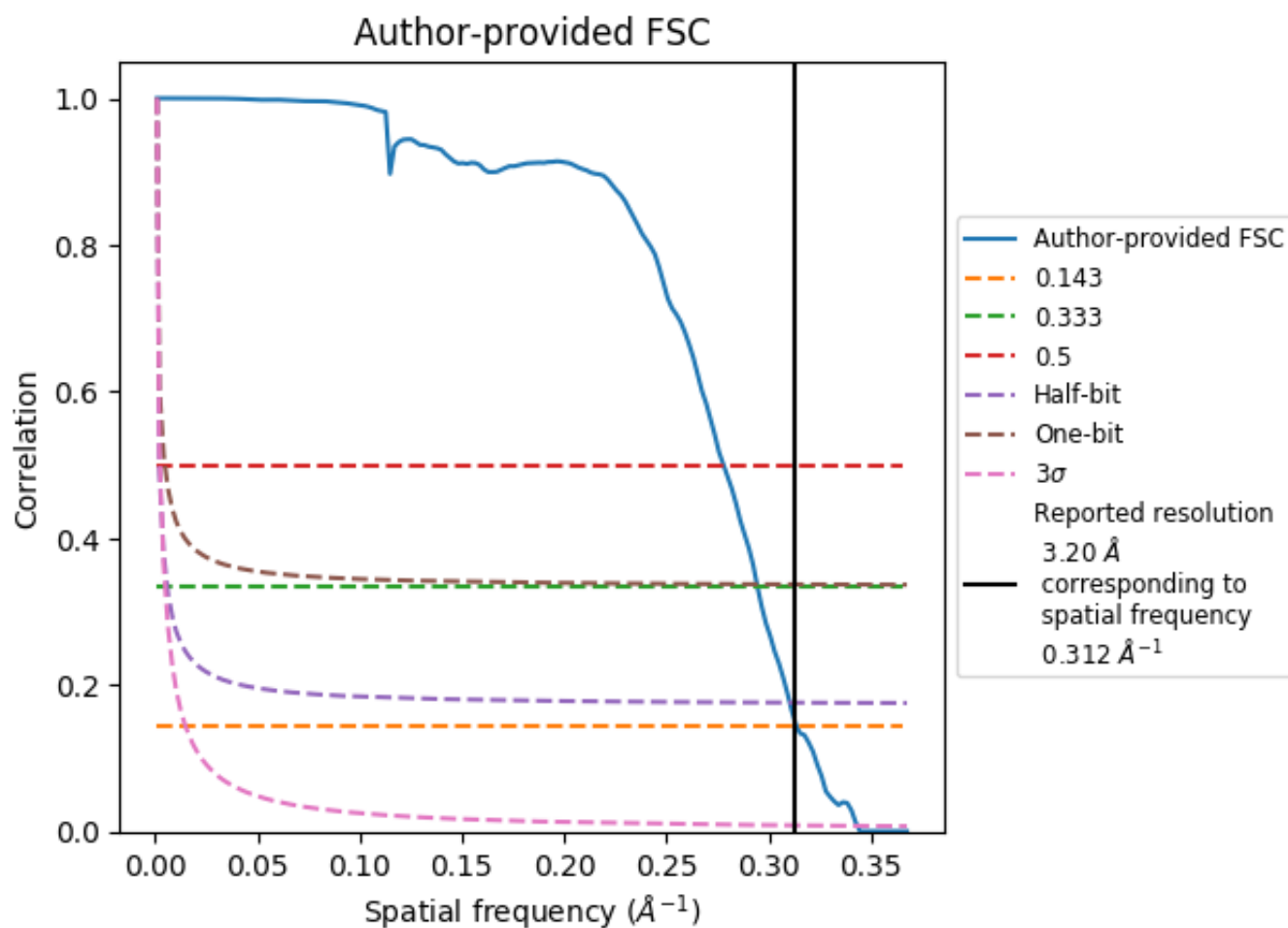
These are global values for the map.

Source	Criterion	Resolution estimate (Å)
Reported value	FSC 0.143 CUT-OFF	3.20
Author-provided FSC	FSC 0.5 CUT-OFF	3.63
Author-provided FSC	FSC 1 BIT CUT-OFF	3.42
Author-provided FSC	FSC 0.33 CUT-OFF	3.42
Author-provided FSC	FSC 1/2 BIT CUT-OFF	3.24
Author-provided FSC	FSC 0.143 CUT-OFF	3.21
Author-provided FSC	FSC 3 SIGMA CUT-OFF	2.93

8.2 Calculated FSC [i](#)

This section was not generated. Half-maps were not provided.

8.3 Author-provided FSC [i](#)

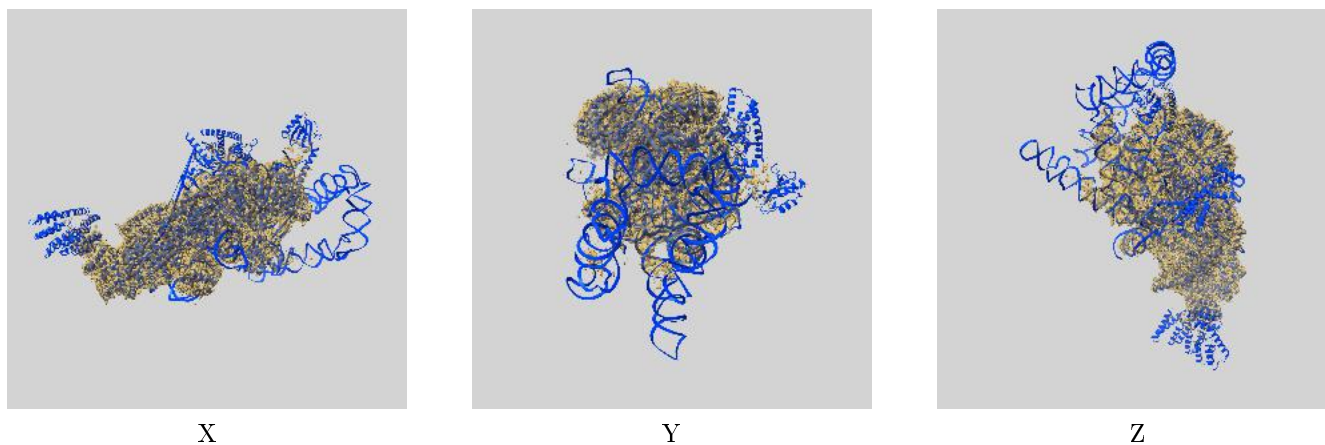


This FSC information was provided by the depositor.

9 Map-model fit [i](#)

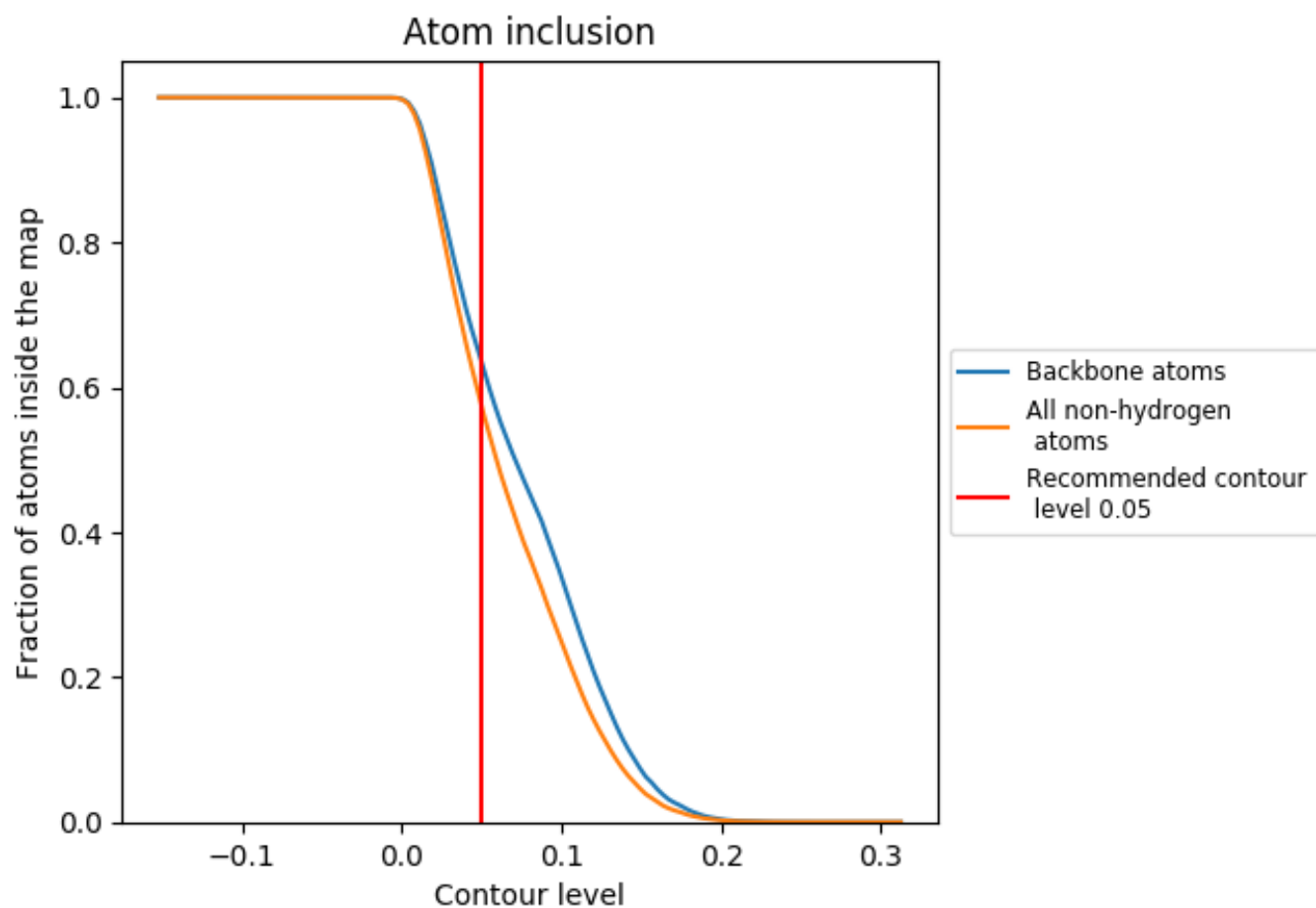
This section contains information regarding the fit between EMDB map EMD-0361 and PDB model 6N7R. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.05 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, 64% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.