



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 04:09 AM UTC

PDB ID : 7NWI / pdb_00007nwi
EMDB ID : EMD-12633
Title : Mammalian pre-termination 80S ribosome with Empty-A site bound by Blasticidin S
Authors : Powers, K.T.; Yadav, S.K.N.; Bufton, J.C.; Schaffitzel, C.
Deposited on : 2021-03-16
Resolution : 3.13 Å(reported)
Based on initial model : 3JAH

This is a Full wwPDB EM Validation 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 : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
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

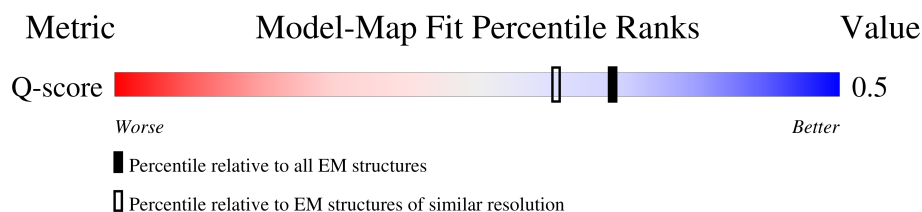
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.13 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	14478 (2.63 - 3.63)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 377740 atoms, of which 160811 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 L8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	244	Total	C	H	N	O	S	0	0
			3819	1169	1955	382	307	6		

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	394	Total	C	H	N	O	S	0	0
			6419	2008	3268	591	539	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 3 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	361	Total	C	H	N	O	S	0	0
			5924	1808	3049	576	477	14		

- Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	292	Total	C	H	N	O	S	0	0
			4805	1509	2419	437	426	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 5 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	236	Total	C	H	N	O	S	0	0
			3931	1215	2033	362	318	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	126	ARG	LYS	conflict	UNP G1SKF7
E	217	GLN	LYS	conflict	UNP G1SKF7

- Molecule 6 is a protein called uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	225	Total	C	H	N	O	S	0	0
			3862	1202	1992	358	301	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	175	ALA	THR	conflict	UNP G1SV32
F	185	GLY	ASN	conflict	UNP G1SV32
F	202	ARG	HIS	conflict	UNP G1SV32
F	233	GLU	GLY	conflict	UNP G1SV32

- Molecule 7 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	237	Total	C	H	N	O	S	0	0
			3954	1213	2051	365	321	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	190	Total	C	H	N	O	S	0	0
			3113	954	1597	284	272	6		

- Molecule 9 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	204	Total	C	H	N	O	S	0	0
			3359	1051	1704	319	272	13		

- Molecule 10 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	169	Total	C	H	N	O	S	0	0
			2739	855	1386	252	240	6		

- Molecule 11 is a protein called L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	L	210	Total	C	H	N	O	S	0	0
			3521	1065	1818	354	280	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	52	SER	ALA	conflict	UNP G1TKB3
L	55	LEU	ILE	conflict	UNP G1TKB3
L	74	ARG	HIS	conflict	UNP G1TKB3
L	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 12 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	M	138	Total	C	H	N	O	S	0	0
			2346	727	1209	221	182	7		

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	N	203	Total	C	H	N	O	S	0	0
			3450	1072	1749	359	266	4		

- Molecule 14 is a protein called L13a.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	O	199	Total	C	H	N	O	S	0	0
			3415	1056	1777	321	256	5		

- Molecule 15 is a protein called L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	P	153	Total	C	H	N	O	S	0	0
			2511	776	1269	241	216	9		

- Molecule 16 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	187	Total	C	H	N	O	S	0	0
			3129	941	1623	311	249	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	77	GLY	ASN	conflict	UNP F6QKI9
Q	86	ILE	VAL	conflict	UNP F6QKI9
Q	106	SER	THR	conflict	UNP F6QKI9

- Molecule 17 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	R	180	Total	C	H	N	O	S	0	0
			3172	933	1664	328	238	9		

- Molecule 18 is a protein called L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	S	175	Total	C	H	N	O	S	0	0
			2948	925	1494	284	235	10		

- Molecule 19 is a protein called eL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	T	159	Total	C	H	N	O	S	0	0
			2664	823	1366	252	217	6		

- Molecule 20 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	U	99	Total	C	H	N	O	S	0	0
			1636	518	828	141	147	2		

- Molecule 21 is a protein called eL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	V	131	Total	C	H	N	O	S	0	0
			2018	618	1039	184	172	5		

- Molecule 22 is a protein called 60S ribosomal protein L24-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	W	63	Total	C	H	N	O	S	0	0
			1069	337	541	103	85	3		

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	X	119	Total	C	H	N	O	S	0	0
			2029	624	1053	183	168	1		

- Molecule 24 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Y	134	Total	C	H	N	O	S	0	0
			2318	700	1203	226	186	3		

- Molecule 25 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 26 is a protein called uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	a	147	Total	C	H	N	O	S	0	0
			2367	734	1205	239	185	4		

- Molecule 27 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	b	75	Total	C	H	N	O	S	0	0
			1259	378	650	130	98	3		

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	c	94	Total	C	H	N	O	S	0	0
			1501	465	769	130	131	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	34	THR	SER	conflict	UNP G1TDL2
c	95	ALA	SER	conflict	UNP G1TDL2

- Molecule 29 is a protein called eL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	d	107	Total	C	H	N	O	S	0	0
			1818	560	930	171	155	2		

- Molecule 30 is a protein called eL32.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	e	128	Total	C	H	N	O	S	0	0
			2200	667	1147	216	165	5		

- Molecule 31 is a protein called eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	f	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	143	4		

- Molecule 32 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	g	114	Total	C	H	N	O	S	0	0
			1907	566	1001	187	147	6		

- Molecule 33 is a protein called uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	h	122	Total	C	H	N	O	S	0	0
			2160	640	1147	204	168	1		

- Molecule 34 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	i	102	Total	C	H	N	O	S	0	0
			1744	520	914	176	129	5		

- Molecule 35 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	j	86	Total	C	H	N	O	S	0	0
			1442	434	737	155	111	5		

- Molecule 36 is a protein called L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	k	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

- Molecule 37 is a protein called ribosomal protein eL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	l	50	Total	C	H	N	O	S	0	0
			927	281	483	98	64	1		

- Molecule 38 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	m	52	Total	C	H	N	O	S	0	0
			894	266	465	90	67	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	54	LEU	ARG	conflict	UNP A0A6P4TG29
m	74	HIS	ARG	conflict	UNP A0A6P4TG29

- Molecule 39 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	n	23	Total	C	H	N	O	S	0	0
			486	134	264	61	25	2		

- Molecule 40 is a protein called LOW QUALITY PROTEIN: 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	o	104	Total	C	H	N	O	S	0	0
			1772	533	921	174	138	6		

- Molecule 41 is a protein called ribosomal protein eL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	p	91	Total	C	H	N	O	S	0	0
			1467	445	759	136	120	7		

- Molecule 42 is a protein called eL28.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	r	125	Total	C	H	N	O	S	0	0
			2061	621	1060	206	168	6		

- Molecule 43 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	s	198	Total	C	H	N	O	S	0	0
			3098	969	1575	265	280	9		

- Molecule 44 is a protein called L12.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	t	163	Total	C	H	N	O	S	0	0
			2533	773	1295	230	230	5		

- Molecule 45 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	AA	208	Total	C	H	N	O	S	0	0
			3288	1045	1646	289	300	8		

- Molecule 46 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	BB	213	Total	C	H	N	O	S	0	0
			3533	1098	1804	309	308	14		

- Molecule 47 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	CC	218	Total	C	H	N	O	S	0	0
			3472	1102	1780	287	296	7		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	61	LEU	ILE	conflict	UNP O55214
CC	73	VAL	MET	conflict	UNP O55214
CC	101	ALA	SER	conflict	UNP O55214
CC	119	ALA	GLY	conflict	UNP O55214
CC	142	LYS	GLU	conflict	UNP O55214
CC	215	LEU	MET	conflict	UNP O55214
CC	227	TRP	ARG	conflict	UNP O55214

- Molecule 48 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	DD	227	Total	C	H	N	O	S	0	0
			3622	1124	1858	317	315	8		

- Molecule 49 is a protein called S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	EE	262	Total	C	H	N	O	S	0	0
			4248	1323	2175	384	357	9		

- Molecule 50 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	FF	191	Total	C	H	N	O	S	0	0
			3072	943	1563	286	273	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FF	0	MET	-	initiating methionine	UNP G1TFM5

- Molecule 51 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	GG	237	Total	C	H	N	O	S	0	0
			4010	1200	2087	387	329	7		

- Molecule 52 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	HH	189	Total	C	H	N	O	S	0	0
			3137	969	1616	280	271	1		

- Molecule 53 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	II	206	Total	C	H	N	O	S	0	0
			3458	1058	1772	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	variant	UNP G1TJW1

- Molecule 54 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	JJ	185	Total	C	H	N	O	S	0	0
			3165	969	1640	306	248	2		

- Molecule 55 is a protein called S10_pectin domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	KK	98	Total	C	H	N	O	S	0	0
			1682	539	855	148	134	6		

- Molecule 56 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	LL	152	Total	C	H	N	O	S	0	0
			2551	788	1313	232	212	6		

- Molecule 57 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	MM	124	Total	C	H	N	O	S	0	0
			1951	600	993	170	179	9		

- Molecule 58 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	NN	150	Total	C	H	N	O	S	0	0
			2502	773	1294	229	205	1		

- Molecule 59 is a protein called S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	OO	136	Total	C	H	N	O	S	0	0
			2055	621	1039	199	190	6		

- Molecule 60 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	PP	127	Total	C	H	N	O	S	0	0
			2180	673	1120	201	179	7		

- Molecule 61 is a protein called Rps16 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	QQ	141	Total	C	H	N	O	S	0	0
			2317	715	1193	212	194	3		

- Molecule 62 is a protein called S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	RR	129	Total	C	H	N	O	S	0	0
			2150	658	1103	193	191	5		

- Molecule 63 is a protein called ribosomal protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	SS	137	Total	C	H	N	O	S	0	0
			2330	714	1191	231	193	1		

- Molecule 64 is a protein called S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	TT	141	Total	C	H	N	O	S	0	0
			2244	692	1142	212	195	3		

- Molecule 65 is a protein called Ribosomal_S10 domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	UU	104	Total	C	H	N	O	S	0	0
			1704	514	883	155	148	4		

- Molecule 66 is a protein called S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	VV	83	Total	C	H	N	O	S	0	0
			1270	394	634	118	119	5		

- Molecule 67 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	WW	129	Total	C	H	N	O	S	0	0
			2114	659	1080	193	176	6		

- Molecule 68 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms						AltConf	Trace
68	XX	141	Total	C	H	N	O	S	0	0
			2265	693	1167	219	183	3		

- Molecule 69 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	YY	126	Total	C	H	N	O	S	0	0
			2113	646	1090	200	172	5		

- Molecule 70 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms						AltConf	Trace
70	ZZ	75	Total	C	H	N	O	S	0	0
			1254	382	656	111	104	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ZZ	3	MET	-	initiating methionine	UNP G1TDB3

- Molecule 71 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	aa	98	Total	C	H	N	O	S	0	0
			1609	486	828	161	129	5		

- Molecule 72 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	bb	83	Total	C	H	N	O	S	0	0
			1323	408	672	121	115	7		

- Molecule 73 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	cc	61	Total	C	H	N	O	S	0	0
			972	290	497	92	91	2		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
cc	5	HIS	ARG	conflict	UNP G1TIB4
cc	18	ILE	LEU	conflict	UNP G1TIB4
cc	20	LYS	ARG	conflict	UNP G1TIB4
cc	40	HIS	ARG	conflict	UNP G1TIB4
cc	42	THR	ILE	conflict	UNP G1TIB4

- Molecule 74 is a protein called ribosomal protein uS14.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	dd	53	Total	C	H	N	O	S	0	0
			883	278	438	90	72	5		

- Molecule 75 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	ee	57	Total	C	H	N	O	S	0	0
			959	282	502	101	73	1		

- Molecule 76 is a protein called S27a.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	ff	62	Total	C	H	N	O	S	0	0
			1057	331	537	98	85	6		

- Molecule 77 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	gg	313	Total	C	H	N	O	S	0	0
			4830	1535	2394	424	465	12		

- Molecule 78 is a protein called Sec61Beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	1	15	Total	C	H	N	O	S	0	0
			242	82	117	20	22	1		

- Molecule 79 is a RNA chain called P-Site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	2	76	Total	C	H	N	O	P	0	0
			2439	723	823	291	527	75		

- Molecule 80 is a RNA chain called 28S ribosomal RNA+BlaS.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	5	3662	Total	C	H	N	O	P	0	0
			118122	34947	39636	14363	25515	3661		

- Molecule 81 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	7	120	Total	C	H	N	O	P	0	0
			3854	1141	1296	456	842	119		

- Molecule 82 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	8	156	Total	C	H	N	O	P	0	0
			4997	1480	1683	585	1094	155		

- Molecule 83 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	9	1719	Total	C	H	N	O	P	0	0
			55209	16371	18529	6586	12005	1718		

- Molecule 84 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	K	10	Total	C	N	O	P	0	0
			217	97	41	69	10		

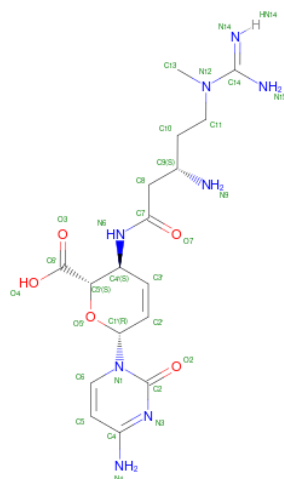
- Molecule 85 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
85	B	2	Total	Mg	0
			2	2	
85	P	1	Total	Mg	0
			1	1	
85	V	1	Total	Mg	0
			1	1	
85	g	1	Total	Mg	0
			1	1	
85	j	1	Total	Mg	0
			1	1	
85	5	159	Total	Mg	0
			159	159	
85	7	5	Total	Mg	0
			5	5	
85	8	1	Total	Mg	0
			1	1	
85	9	39	Total	Mg	0
			39	39	

- Molecule 86 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
86	g	1	Total	Zn	0
			1	1	
86	j	1	Total	Zn	0
			1	1	
86	m	1	Total	Zn	0
			1	1	
86	o	1	Total	Zn	0
			1	1	
86	p	1	Total	Zn	0
			1	1	

- Molecule 87 is BLASTICIDIN S (CCD ID: BLS) (formula: C₁₇H₂₆N₈O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
87	5	1	Total	C	H	N	O	0
			55	17	25	8	5	

MolProbit failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.92	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	79000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 216 ligands modelled in this entry, 215 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
87	BLS	5	5241	-	30,31,31	4.20	16 (53%)	30,43,43	1.61	8 (26%)

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
87	BLS	5	5241	-	-	2/25/38/38	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	5	5241	BLS	O5'-C1'	11.37	1.65	1.42
87	5	5241	BLS	O5'-C5'	-10.24	1.23	1.43
87	5	5241	BLS	C3'-C2'	7.33	1.55	1.33
87	5	5241	BLS	C4'-C5'	6.62	1.68	1.53
87	5	5241	BLS	C1'-N1	-5.59	1.40	1.48
87	5	5241	BLS	C7-N6	4.94	1.44	1.34
87	5	5241	BLS	C1'-C2'	-4.51	1.38	1.49
87	5	5241	BLS	C14-N12	4.39	1.44	1.35
87	5	5241	BLS	C14-N15	4.37	1.44	1.34
87	5	5241	BLS	C4-N4	4.34	1.44	1.33
87	5	5241	BLS	C5-C4	-3.89	1.33	1.42
87	5	5241	BLS	C6-N1	-2.84	1.31	1.38
87	5	5241	BLS	O2-C2	-2.73	1.18	1.23
87	5	5241	BLS	C4'-C3'	-2.71	1.40	1.49
87	5	5241	BLS	O7-C7	-2.38	1.18	1.23
87	5	5241	BLS	C2-N1	-2.34	1.35	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	5	5241	BLS	C3'-C4'-N6	-3.35	104.28	110.44
87	5	5241	BLS	C8-C7-N6	3.08	120.46	116.25
87	5	5241	BLS	C1'-N1-C2	2.95	122.42	117.94
87	5	5241	BLS	N15-C14-N12	2.34	121.20	118.64
87	5	5241	BLS	C1'-C2'-C3'	-2.28	119.64	122.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	5	5241	BLS	C11-C10-C9	-2.27	109.29	113.96
87	5	5241	BLS	N4-C4-N3	2.23	121.90	117.91
87	5	5241	BLS	C1'-N1-C6	-2.12	117.95	121.06

There are no chirality outliers.

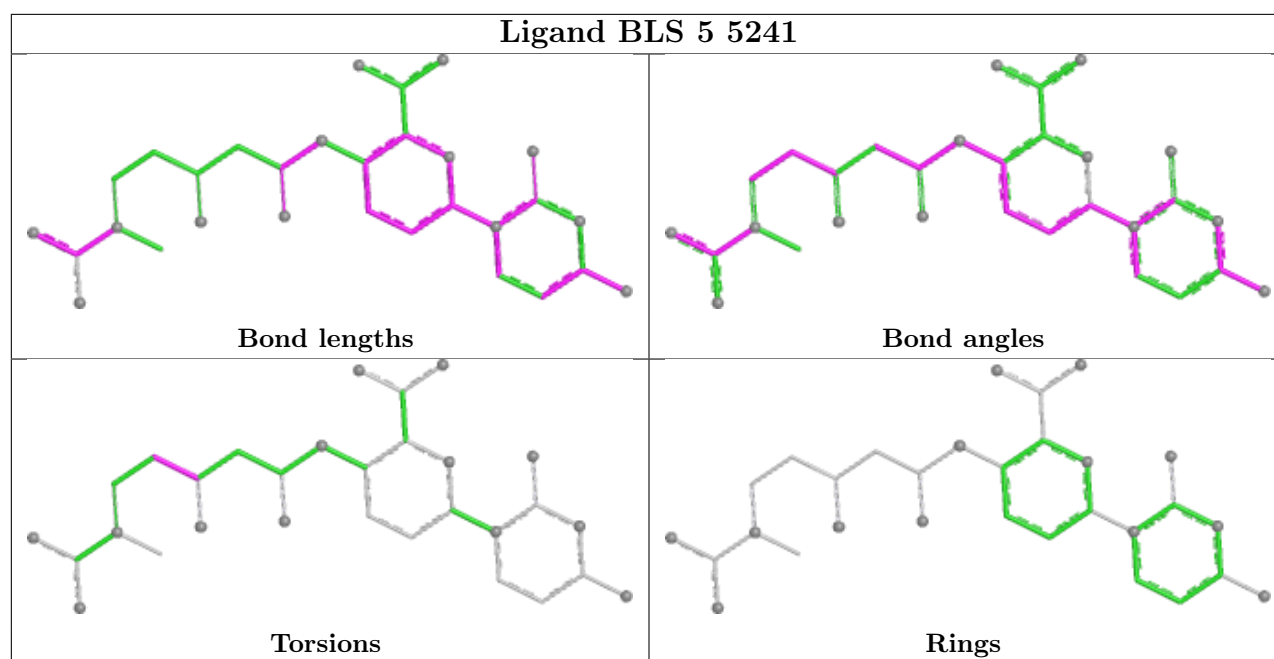
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
87	5	5241	BLS	C11-C10-C9-C8
87	5	5241	BLS	C11-C10-C9-N9

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.



4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
76	ff	1
80	5	1
79	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	ff	118:SER	C	126:PHE	N	14.56
1	5	2016:C	O3'	2017:A	P	7.36
1	2	16:C	O3'	18:G	P	6.49

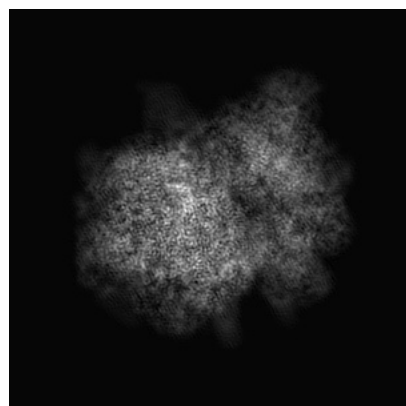
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12633. These allow visual inspection of the internal detail of the map and identification of artifacts.

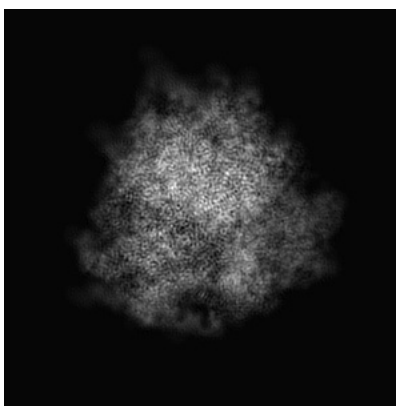
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

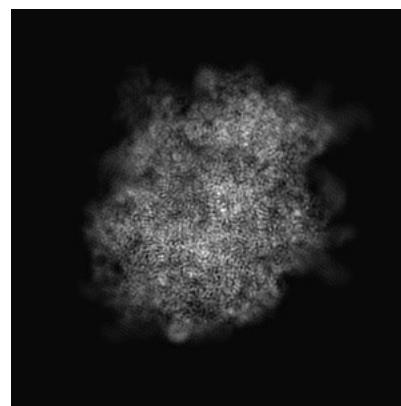
5.1.1 Primary map



X

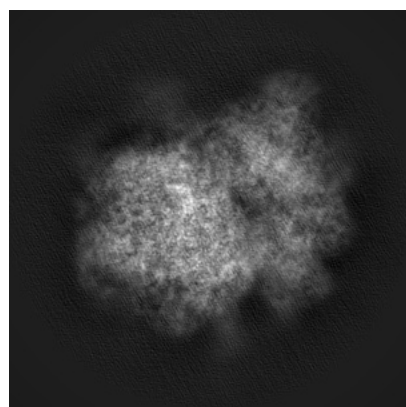


Y

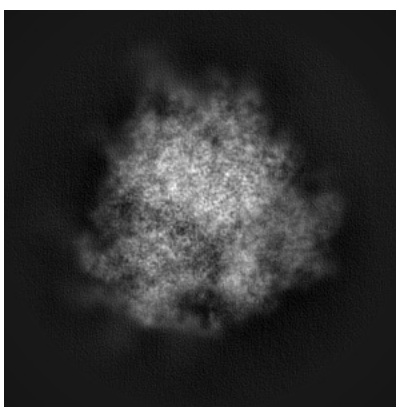


Z

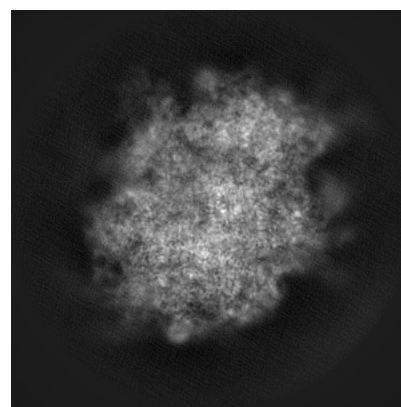
5.1.2 Raw map



X



Y

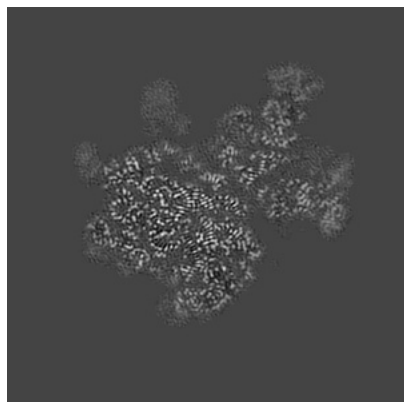


Z

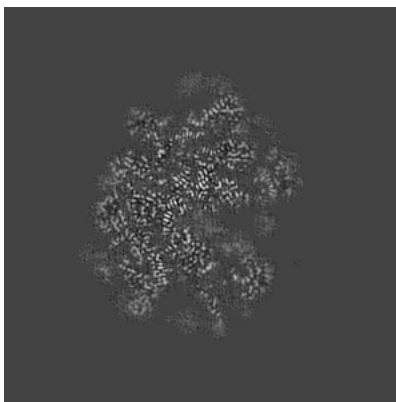
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

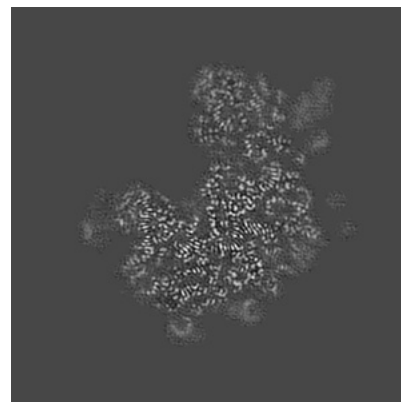
5.2.1 Primary map



X Index: 150

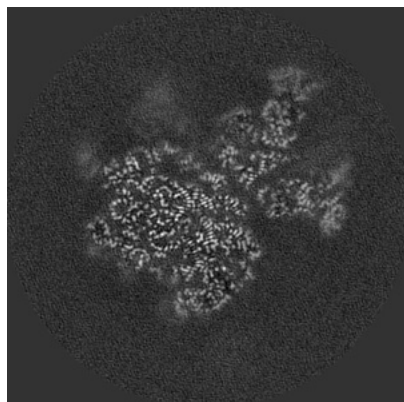


Y Index: 150

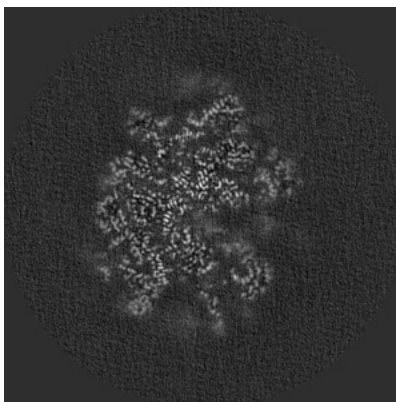


Z Index: 150

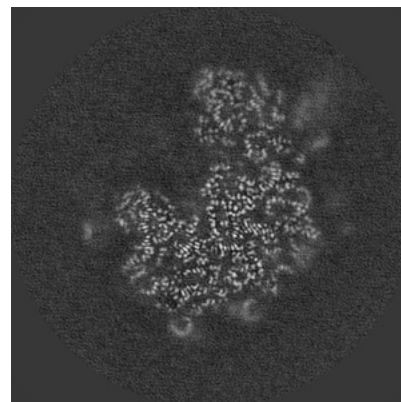
5.2.2 Raw map



X Index: 150



Y Index: 150

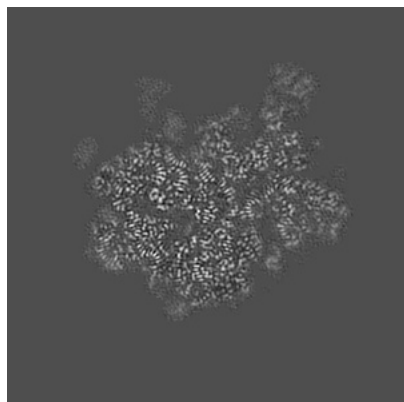


Z Index: 150

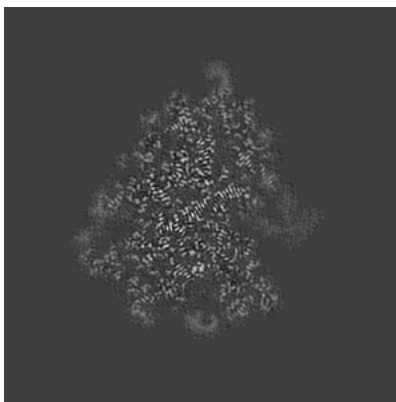
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

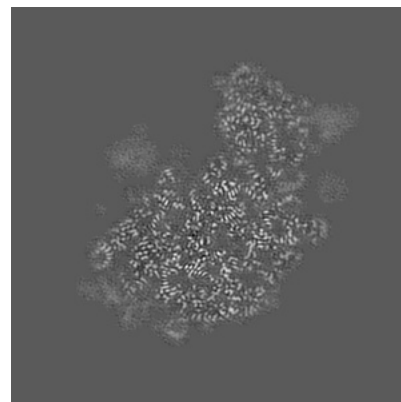
5.3.1 Primary map



X Index: 158

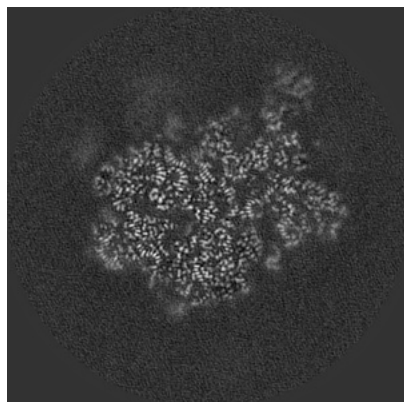


Y Index: 130

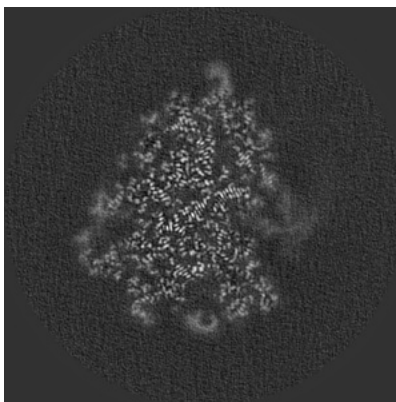


Z Index: 126

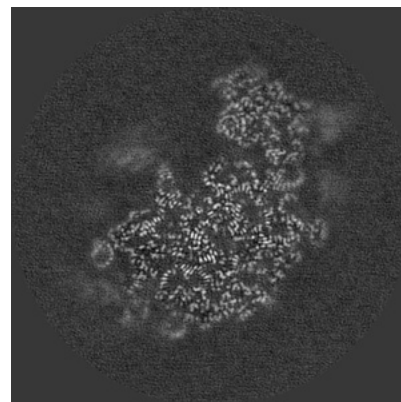
5.3.2 Raw map



X Index: 158



Y Index: 130

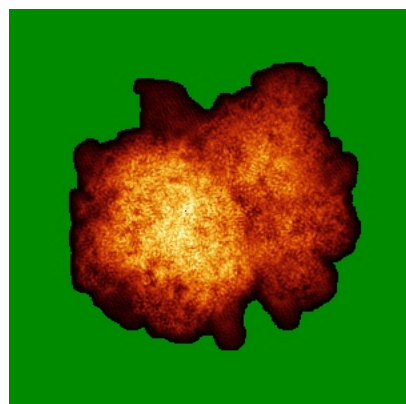


Z Index: 128

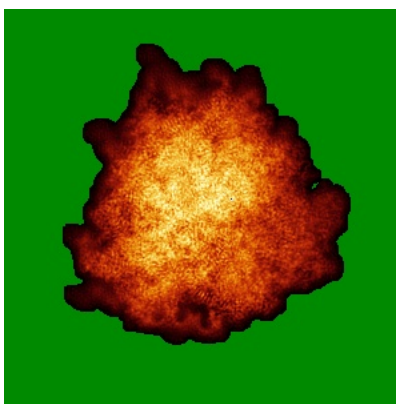
The images above show the largest variance slices of the map in three orthogonal directions.

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

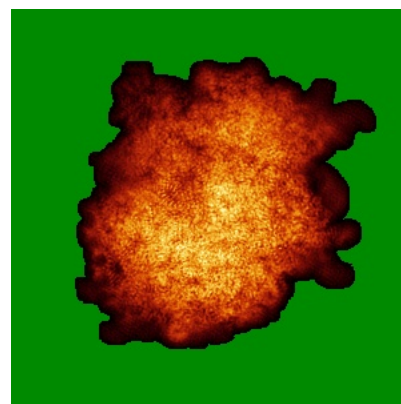
5.4.1 Primary map



X

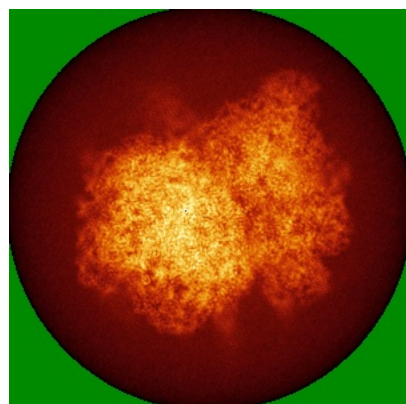


Y

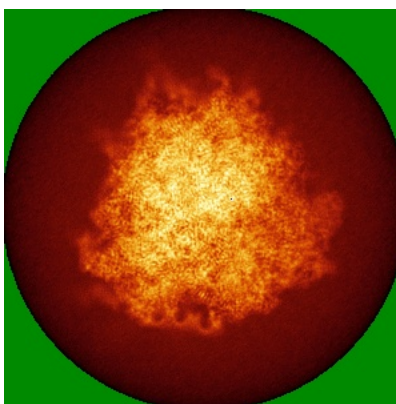


Z

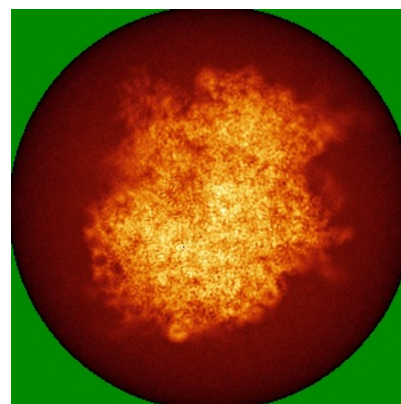
5.4.2 Raw map



X



Y

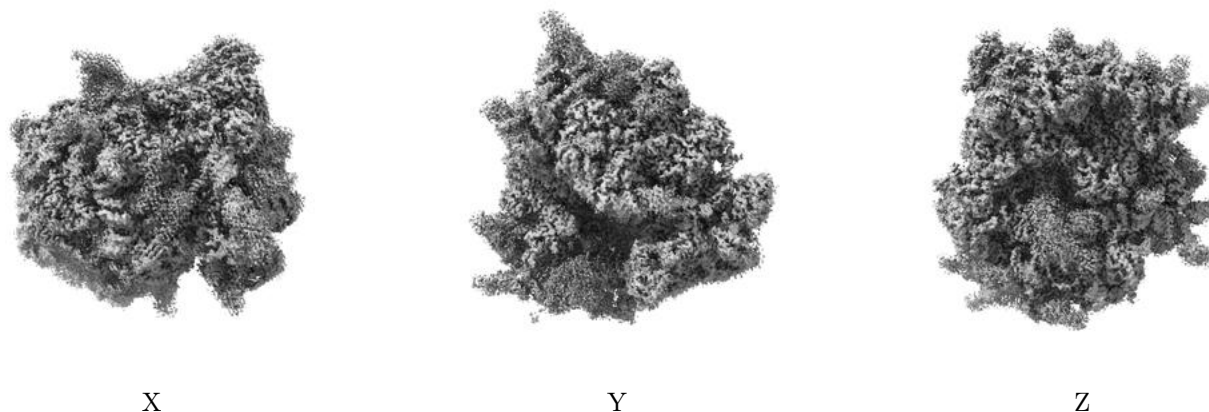


Z

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.

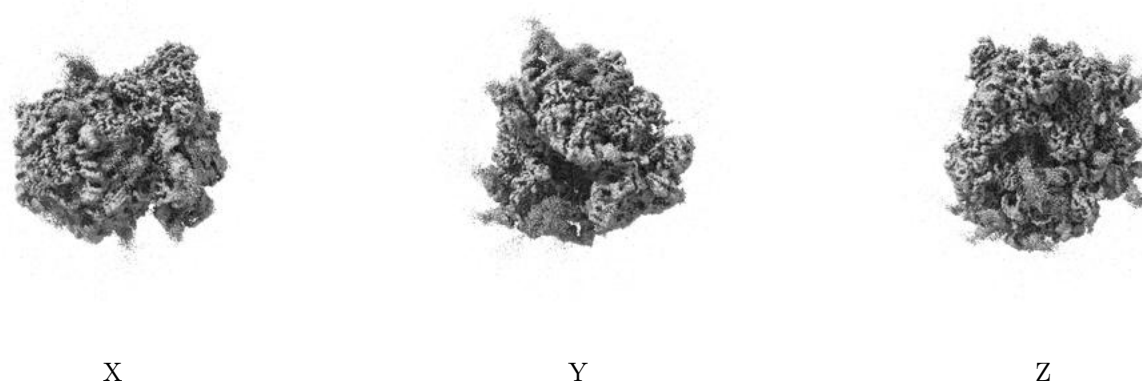
5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

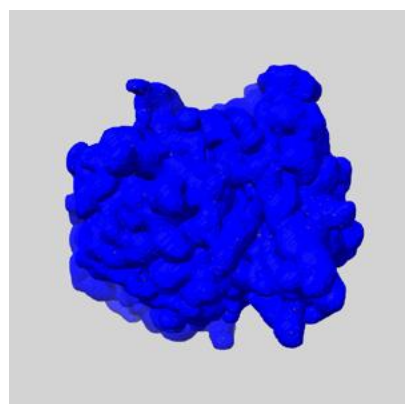
5.6 Mask visualisation [i](#)

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

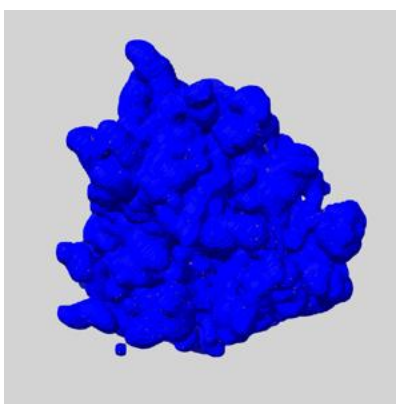
A mask typically either:

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

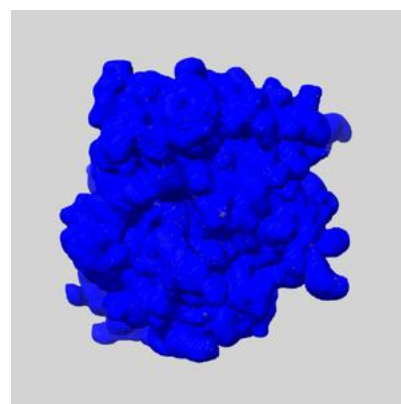
5.6.1 emd_12633_msk_1.map [i](#)



X



Y

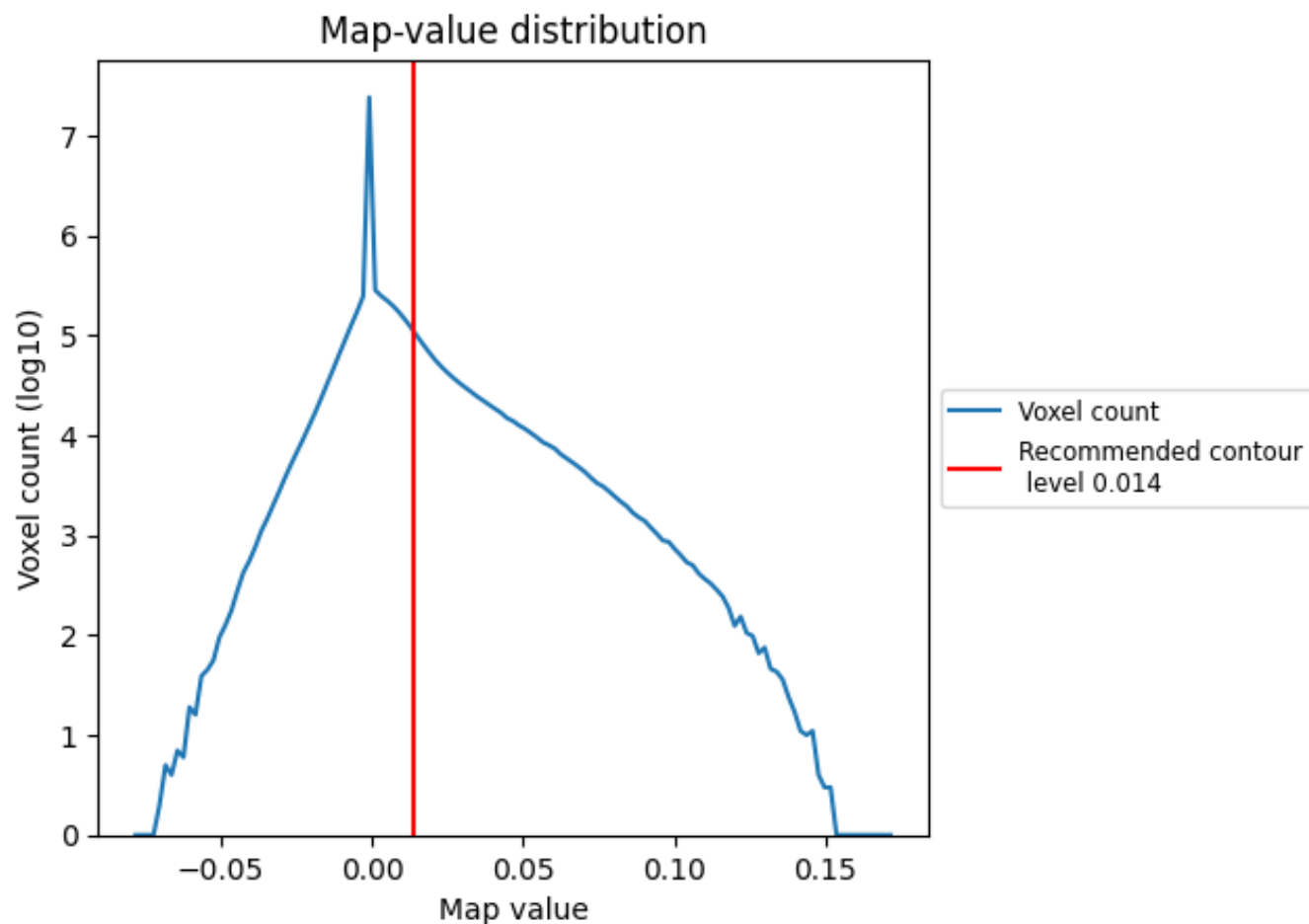


Z

6 Map analysis [i](#)

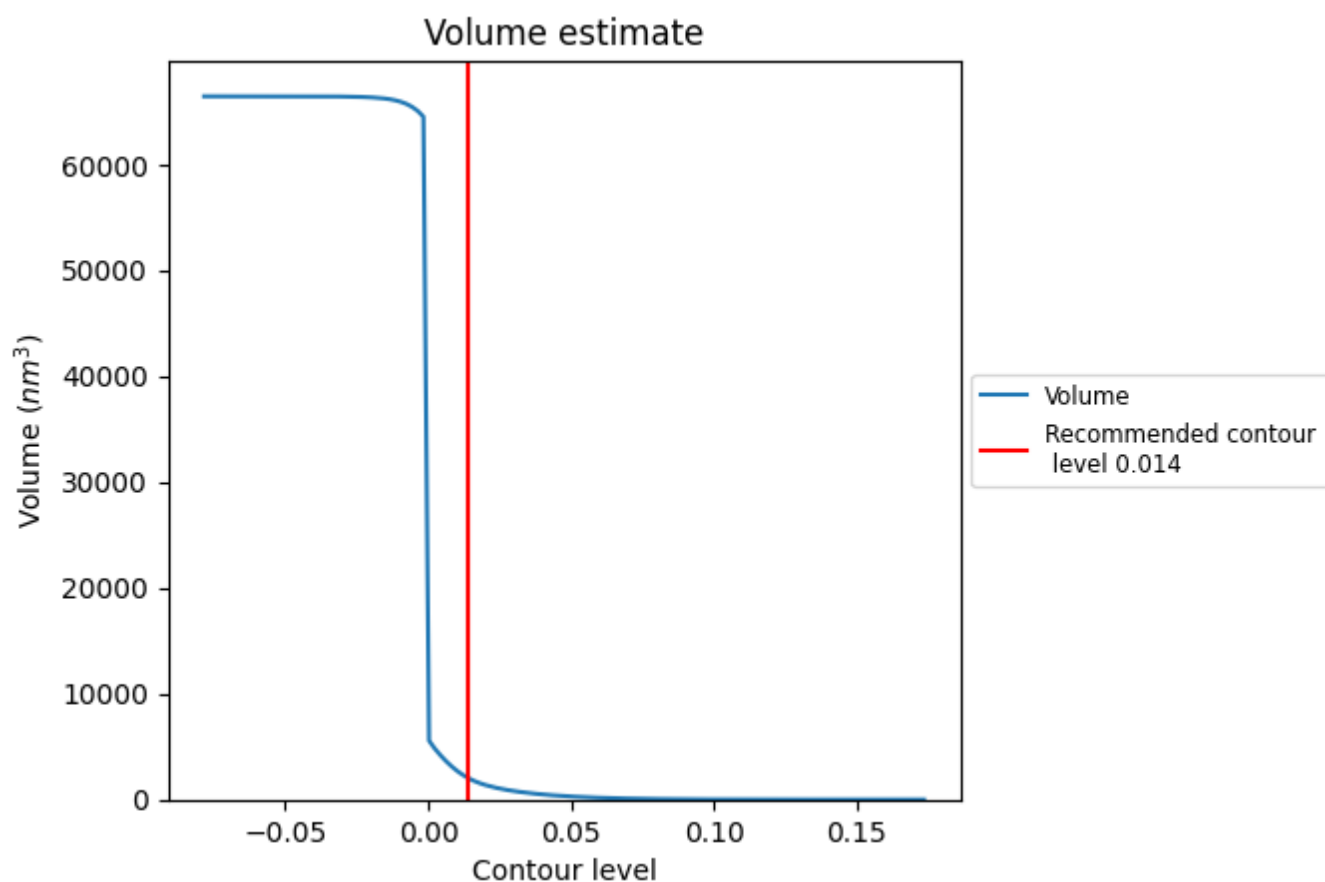
This section contains the results of statistical analysis of the map.

6.1 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.

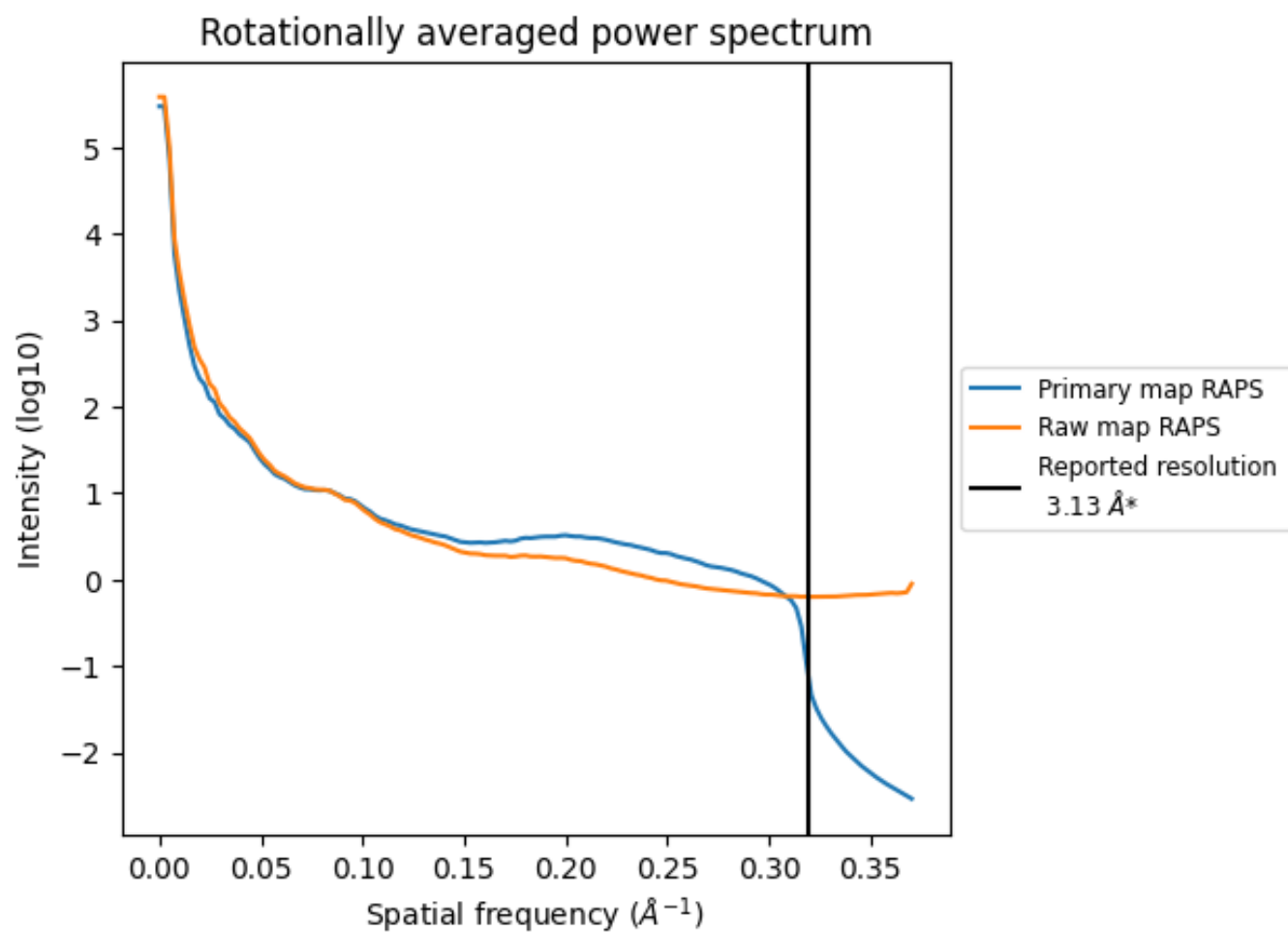
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 2047 nm³; this corresponds to an approximate mass of 1850 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.

6.3 Rotationally averaged power spectrum ⓘ

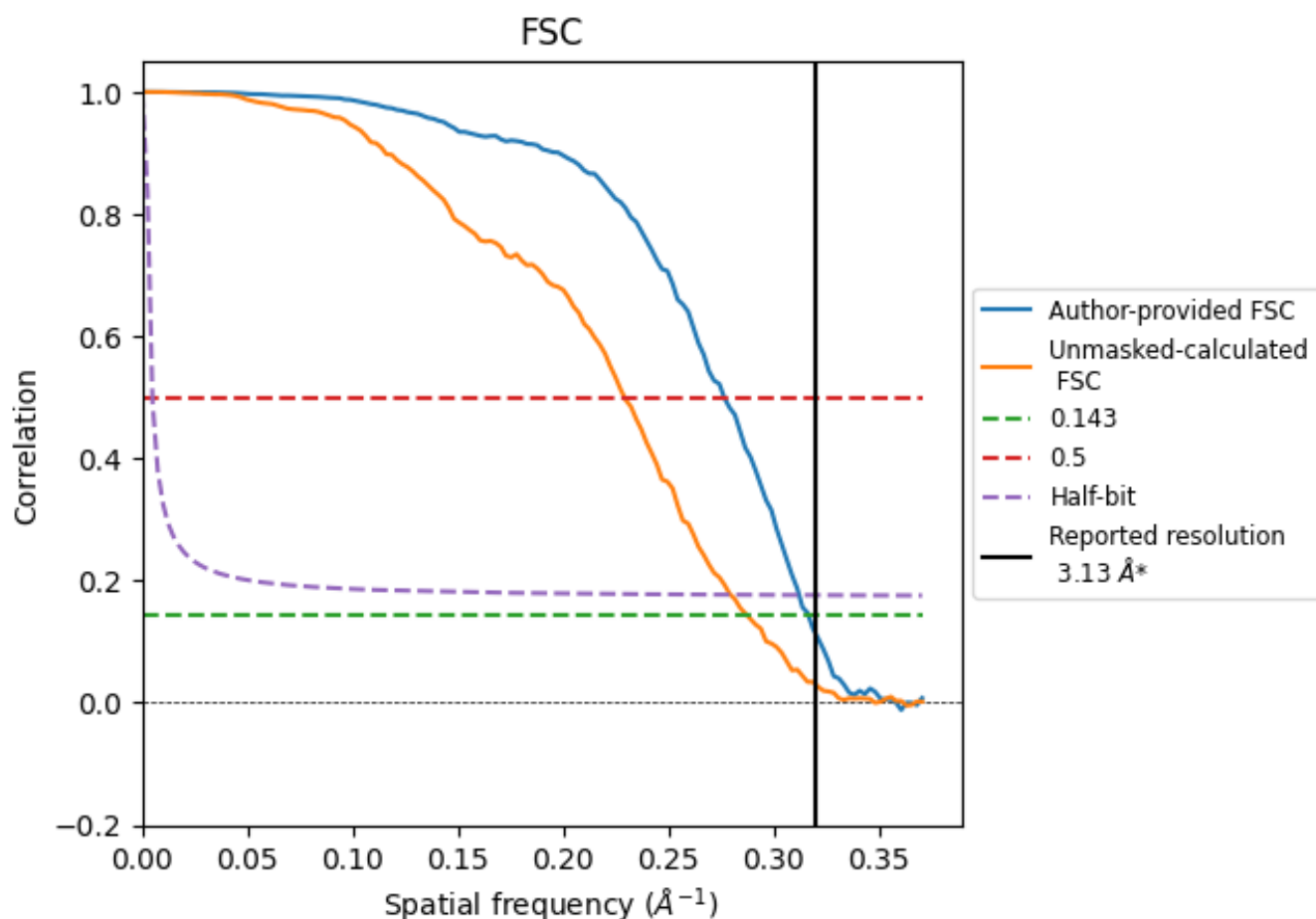


*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.319 $\text{\AA}^{-1}$

7.2 Resolution estimates [i](#)

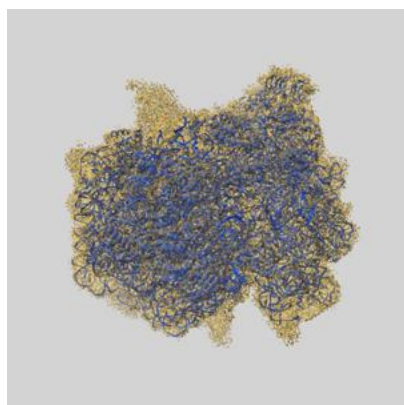
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	3.16	3.62	3.21
Unmasked-calculated*	3.48	4.37	3.58

*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 3.48 differs from the reported value 3.13 by more than 10 %

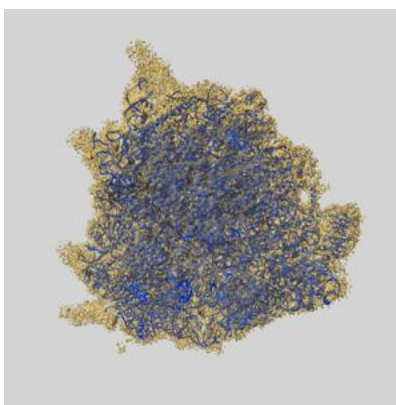
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12633 and PDB model 7NWI. Per-residue inclusion information can be found in section ?? on page ??.

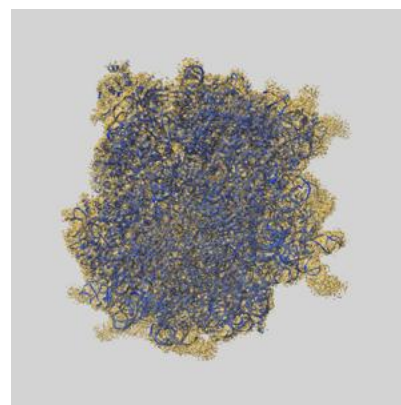
8.1 Map-model overlay [i](#)



X



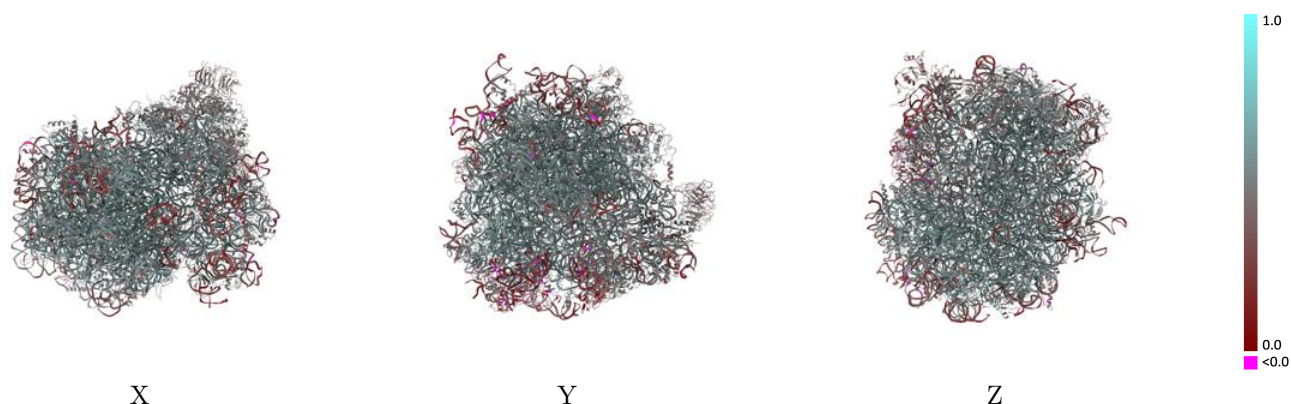
Y



Z

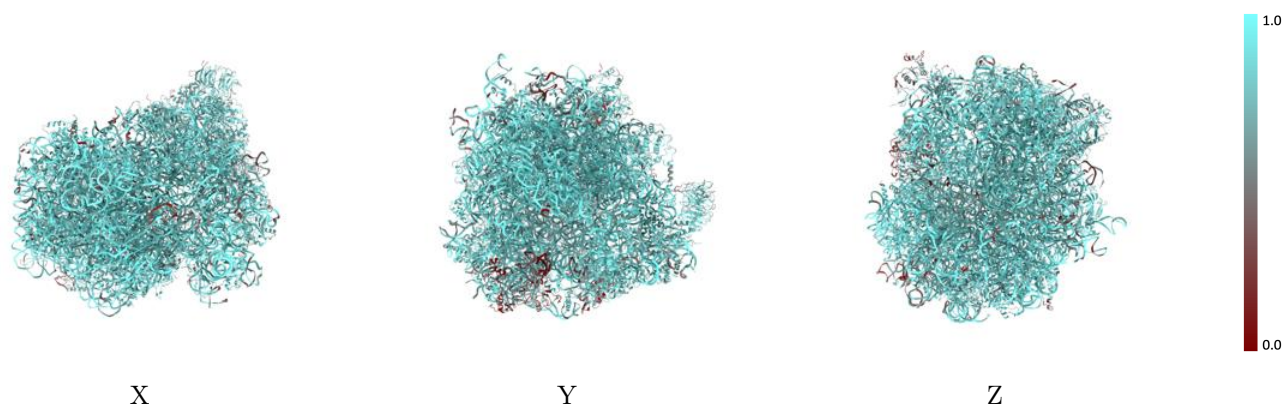
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



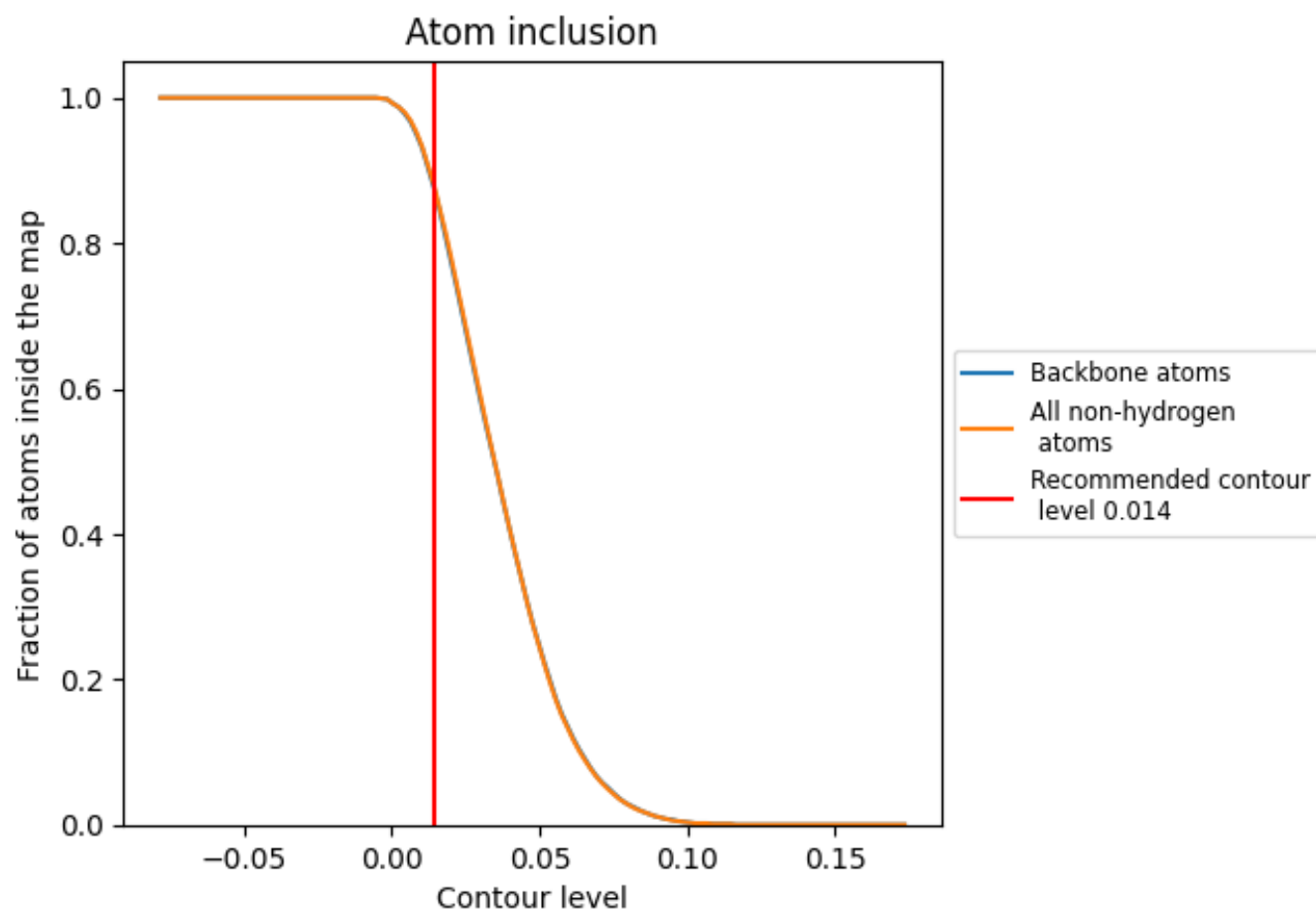
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 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 (0.014).

8.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8830	 0.5000
1	 0.7360	 0.4870
2	 0.8280	 0.4300
5	 0.9190	 0.5060
7	 0.9910	 0.5660
8	 0.9590	 0.5380
9	 0.9320	 0.4910
A	 0.9310	 0.5760
AA	 0.8530	 0.4950
B	 0.9160	 0.5500
BB	 0.8440	 0.4880
C	 0.9080	 0.5510
CC	 0.8670	 0.5180
D	 0.8940	 0.5240
DD	 0.7400	 0.4290
E	 0.8330	 0.4990
EE	 0.8590	 0.5120
F	 0.8930	 0.5530
FF	 0.8110	 0.4780
G	 0.8070	 0.4810
GG	 0.7940	 0.4230
H	 0.8830	 0.5350
HH	 0.7460	 0.4360
I	 0.9030	 0.5500
II	 0.8530	 0.5030
J	 0.8710	 0.4990
JJ	 0.8460	 0.4930
K	 0.5710	 0.4100
KK	 0.7810	 0.4160
L	 0.8500	 0.5100
LL	 0.8160	 0.5080
M	 0.8920	 0.5310
MM	 0.4510	 0.2860
N	 0.9330	 0.5700
NN	 0.8550	 0.5060



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
O	 0.9070	 0.5570
OO	 0.8470	 0.5040
P	 0.9050	 0.5600
PP	 0.7460	 0.4050
Q	 0.9060	 0.5600
QQ	 0.8430	 0.4680
R	 0.8810	 0.5240
RR	 0.7640	 0.4470
S	 0.9160	 0.5640
SS	 0.8160	 0.4530
T	 0.9030	 0.5400
TT	 0.8340	 0.4640
U	 0.8460	 0.4820
UU	 0.7290	 0.4290
V	 0.9090	 0.5510
VV	 0.8260	 0.4840
W	 0.8900	 0.5310
WW	 0.8850	 0.5300
X	 0.8980	 0.5340
XX	 0.8830	 0.5340
Y	 0.8900	 0.5350
YY	 0.8420	 0.4620
Z	 0.8910	 0.5270
ZZ	 0.7510	 0.4360
a	 0.9210	 0.5690
aa	 0.8830	 0.5220
b	 0.7940	 0.4880
bb	 0.7950	 0.4870
c	 0.8880	 0.5380
cc	 0.7850	 0.4770
d	 0.8730	 0.5300
dd	 0.8920	 0.5080
e	 0.9040	 0.5700
ee	 0.7270	 0.4550
f	 0.9410	 0.5780
ff	 0.6060	 0.2720
g	 0.8900	 0.5400
gg	 0.7550	 0.4120
h	 0.8650	 0.5270
i	 0.8580	 0.5110
j	 0.9440	 0.5730
k	 0.8130	 0.4880

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
l	 0.9120	 0.5500
m	 0.8850	 0.5480
n	 0.8560	 0.5390
o	 0.8920	 0.5430
p	 0.8690	 0.5470
r	 0.8970	 0.5510
s	 0.2220	 0.1370
t	 0.1840	 0.1670