



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:20 PM UTC

PDB ID : 7A5I / pdb_00007a5i
EMDB ID : EMD-11644
Title : Structure of the human mitoribosome with A- P-and E-site mt-tRNAs
Authors : Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on : 2020-08-21
Resolution : 3.70 Å(reported)

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

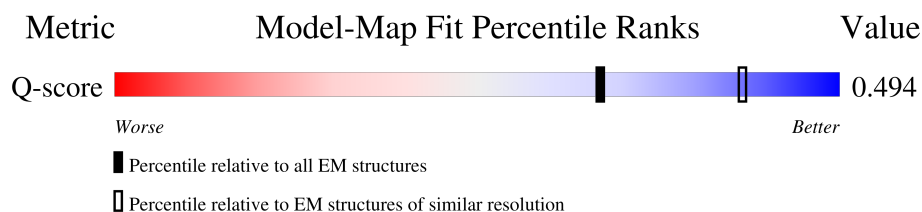
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 163843 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 nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Y2	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 2 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A3	1485	Total	C	N	O	P	0	0
			31529	14146	5687	10211	1485		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	3107	U	UNK	conflict	GB 1025814679

- Molecule 3 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B3	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 4 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D3	236	Total	C	N	O	S	0	0
			1842	1145	373	315	9		

- Molecule 5 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E3	300	Total	C	N	O	S	0	0
			2365	1523	410	422	10		

- Molecule 6 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F3	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 7 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H3	95	Total	C	N	O	S	0	0
			784	498	152	134			

- Molecule 8 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I3	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 9 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J3	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 10 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K3	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 11 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L3	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 12 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M3	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 13 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N3	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 14 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O3	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 15 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P3	133	Total	C	N	O	S	0	0
			1080	677	209	189	5		

- Molecule 16 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q3	219	Total	C	N	O	S	0	0
			1822	1168	322	323	9		

- Molecule 17 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R3	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 18 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S3	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 19 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T3	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 20 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U3	111	Total	C	N	O	S	0	0
			922	591	176	153	2		

- Molecule 21 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V3	189	Total	C	N	O	S	0	0
			1551	987	278	278	8		

- Molecule 22 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W3	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

- Molecule 23 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X3	243	Total	C	N	O	S	0	0
			2027	1310	350	362	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X3	148	ALA	THR	conflict	UNP Q13084
X3	149	SER	PRO	conflict	UNP Q13084
X3	150	GLY	LYS	conflict	UNP Q13084

- Molecule 24 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y3	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 25 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z3	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 26 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	03	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 27 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	13	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 28 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	23	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

- Molecule 29 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	33	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 30 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	43	36	Total	C	N	O	S	0	0
			322	203	70	46	3		

- Molecule 31 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	53	376	Total	C	N	O	S	0	0
			3064	1987	529	538	10		

- Molecule 32 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	63	325	Total	C	N	O	S	0	0
			2636	1692	465	470	9		

- Molecule 33 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	73	266	Total	C	N	O	S	0	0
			2158	1383	371	388	16		

- Molecule 34 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	83	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 35 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	93	109	Total	C	N	O	S	0	0
			873	565	152	154	2		

- Molecule 36 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	a3	82	Total	C	N	O	S	0	0
			686	434	124	123	5		

- Molecule 37 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	b3	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 38 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c3	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 39 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d3	162	Total	C	N	O	S	0	0
			1347	870	234	235	8		

- Molecule 40 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e3	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 41 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f3	131	Total	C	N	O	S	0	0
			1039	663	169	203	4		

- Molecule 42 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g3	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 43 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h3	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 44 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	i3	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 45 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	j3	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 46 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	k3	84	Total	C	N	O	S	0	0
			655	407	122	121	5		

- Molecule 47 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	l3	23	Total	C	N	O	0	0
			221	137	52	32		

- Molecule 48 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	m3	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 49 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o3	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 50 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	p3	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 51 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	q3	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 52 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	r3	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	s3	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 54 is a protein called Unknown protein/protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	t3	28	Total	C	N	O	0	0
			140	84	28	28		
54	A5	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 55 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B6	217	Total	C	N	O	S	0	0
			1768	1131	321	306	10		

- Molecule 56 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	C6	132	Total	C	N	O	S	0	0
			1082	699	195	184	4		

- Molecule 57 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	D6	322	Total	C	N	O	S	0	0
			2557	1611	476	457	13		

- Molecule 58 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	E6	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 59 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	F6	201	Total	C	N	O	S	0	0
			1668	1069	305	283	11		

- Molecule 60 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	G6	305	Total	C	N	O	S	0	0
			2516	1599	448	455	14		

- Molecule 61 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	H6	122	Total	C	N	O	S	0	0
			999	643	168	185	3		

- Molecule 62 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	I6	136	Total	C	N	O	S	0	0
			1011	637	192	178	4		

- Molecule 63 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	J6	108	Total	C	N	O	S	0	0
			838	521	169	142	6		

- Molecule 64 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	K6	101	Total	C	N	O	S	0	0
			861	537	179	140	5		

- Molecule 65 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	L6	164	Total	C	N	O	S	0	0
			1382	883	257	235	7		

- Molecule 66 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	M6	116	Total	C	N	O	S	0	0
			920	582	182	150	6		

- Molecule 67 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	N6	107	Total	C	N	O	S	0	0
			846	549	153	141	3		

- Molecule 68 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	O6	185	Total	C	N	O	S	0	0
			1528	970	285	267	6		

- Molecule 69 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	P6	96	Total	C	N	O	S	0	0
			774	498	133	135	8		

- Molecule 70 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Q6	86	Total	C	N	O	S	0	0
			740	458	150	124	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q6	50	ARG	CYS	conflict	UNP P82921

- Molecule 71 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	R6	242	Total	C	N	O	S	0	0
			2008	1285	343	372	8		

- Molecule 72 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	S6	126	Total	C	N	O	S	0	0
			1042	673	183	185	1		

- Molecule 73 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	T6	162	Total	C	N	O	S	0	0
			1330	850	231	238	11		

- Molecule 74 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	U6	173	Total	C	N	O	S	0	0
			1461	900	294	263	4		

- Molecule 75 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	V6	328	Total	C	N	O	S	0	0
			2702	1737	452	502	11		

- Molecule 76 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	W6	97	Total	C	N	O	S	0	0
			766	486	137	139	4		

- Molecule 77 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	X6	316	Total	C	N	O	S	0	0
			2531	1625	440	455	11		

- Molecule 78 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Y6	108	Total	C	N	O	S	0	0
			914	593	150	169	2		

- Molecule 79 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Z6	87	Total	C	N	O	S	0	0
			740	473	133	130	4		

- Molecule 80 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	a6	201	Total	C	N	O	S	0	0
			1684	1065	322	292	5		

- Molecule 81 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	b6	256	Total	C	N	O	S	0	0
			2076	1321	350	395	10		

- Molecule 82 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	c6	116	Total	C	N	O	S	0	0
			925	574	181	162	8		

- Molecule 83 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	d6	69	Total	C	N	O	S	0	0
			610	393	130	86	1		

- Molecule 84 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	e6	414	Total	C	N	O	S	0	0
			2838	1805	490	529	14		

- Molecule 85 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	A6	928	Total	C	N	O	P	0	0
			19716	8840	3560	6388	928		

- Molecule 86 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	i4	9	Total	C	N	O	P	0	0
			196	88	39	60	9		

- Molecule 87 is a RNA chain called mt-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	99	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		
87	94	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		

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Mol	Chain	Residues	Atoms					AltConf	Trace
87	X	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A3	96	Total	Mg	0
			96	96	
88	D3	1	Total	Mg	0
			1	1	
88	g3	1	Total	Mg	0
			1	1	
88	o3	1	Total	Mg	0
			1	1	
88	G6	1	Total	Mg	0
			1	1	
88	A6	27	Total	Mg	0
			27	27	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	03	1	Total	Zn	0
			1	1	
89	43	1	Total	Zn	0
			1	1	
89	r3	1	Total	Zn	0
			1	1	
89	B6	1	Total	Zn	0
			1	1	
89	O6	1	Total	Zn	0
			1	1	
89	P6	1	Total	Zn	0
			1	1	
89	T6	1	Total	Zn	0
			1	1	

- Molecule 90 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
90	A5	1	Total	Cl	0
			1	1	

- # GDP
-
- The image displays the chemical structure of Guanosine Diphosphate (GDP). The structure consists of a guanine base, a ribose sugar, and two phosphate groups. The guanine base is a purine derivative with a carbonyl group at C6 and an amino group at C2. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are linked in a diphosphate chain, with the first phosphate attached to the 5' carbon of the ribose. The structure is labeled with various atom identifiers: N1, N2, N3, N7, N9 for nitrogen atoms; C2, C4, C5, C6, C8 for carbon atoms in the guanine base; C1(P), C2(P), C3(S), C4(S), C5' for carbon atoms in the ribose sugar; and O1A, O1B, O2A, O2B, O3A, O3B for oxygen atoms in the phosphate groups. The labels are color-coded: blue for nitrogen atoms, black for carbon atoms, and red for oxygen atoms.

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

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37415	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.501	Depositor
Minimum map value	-0.303	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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 136 ligands modelled in this entry, 135 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	$\# Z > 2$
91	GDP	X6	500	-	29,30,30	1.13	3 (10%)	45,47,47	1.93	11 (24%)

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
91	GDP	X6	500	-	-	6/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	X6	500	GDP	C5-C4	3.18	1.47	1.38
91	X6	500	GDP	C6-N1	-2.57	1.34	1.38
91	X6	500	GDP	C5-N7	-2.15	1.34	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	X6	500	GDP	C5-C4-N3	-6.53	117.99	128.39
91	X6	500	GDP	N9-C4-N3	5.22	136.40	125.95
91	X6	500	GDP	C2-N3-C4	4.90	120.73	112.30
91	X6	500	GDP	C2'-C1'-N9	-3.32	104.00	113.25
91	X6	500	GDP	C3'-C2'-C1'	2.58	106.35	101.46
91	X6	500	GDP	O4'-C1'-N9	2.41	113.81	108.36
91	X6	500	GDP	C6-C5-N7	2.34	134.54	130.29
91	X6	500	GDP	O2B-PB-O3A	2.25	112.17	104.64
91	X6	500	GDP	O6-C6-C5	-2.22	120.67	126.53
91	X6	500	GDP	C4-C5-N7	-2.21	107.17	110.67
91	X6	500	GDP	C1'-N9-C8	-2.04	120.95	126.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	X6	500	GDP	C5'-O5'-PA-O3A

Continued on next page...

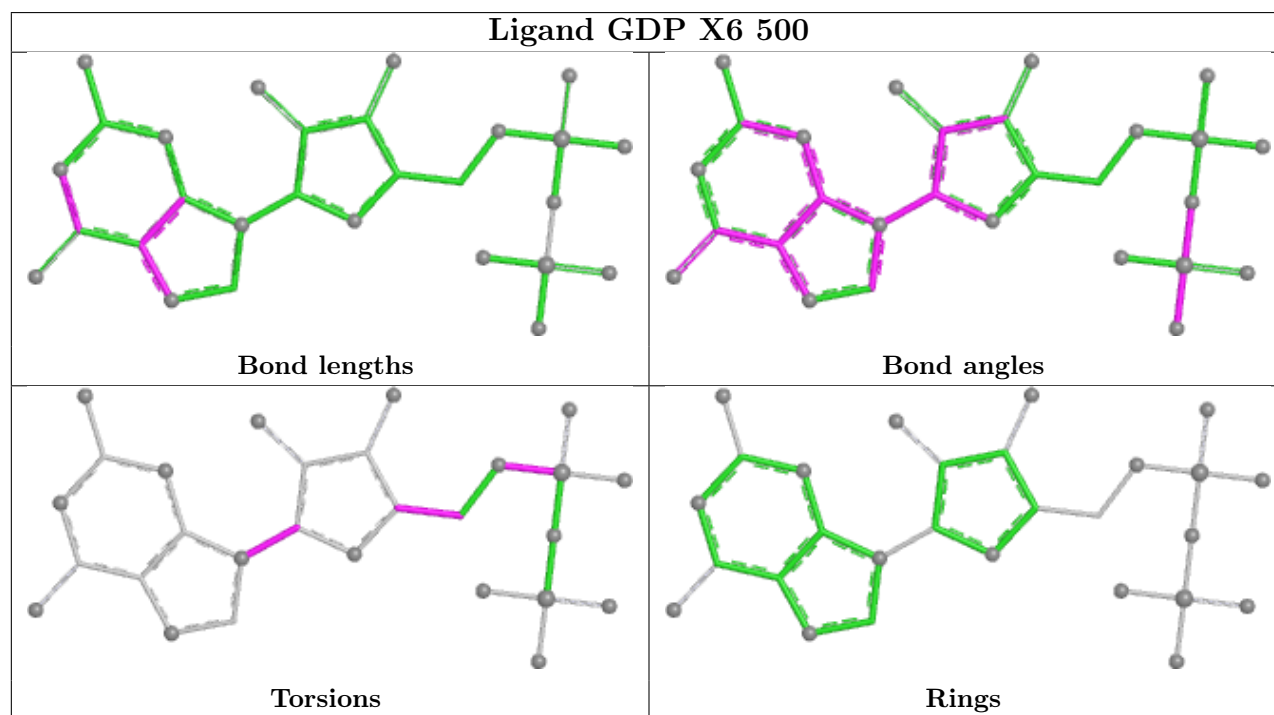
Continued from previous page...

Mol	Chain	Res	Type	Atoms
91	X6	500	GDP	O4'-C1'-N9-C4
91	X6	500	GDP	C3'-C4'-C5'-O5'
91	X6	500	GDP	O4'-C1'-N9-C8
91	X6	500	GDP	O4'-C4'-C5'-O5'
91	X6	500	GDP	C5'-O5'-PA-O1A

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
18	S3	1
23	X3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S3	57:SER	C	58:SER	N	1.18
1	X3	5:LYS	C	6:TYR	N	1.15

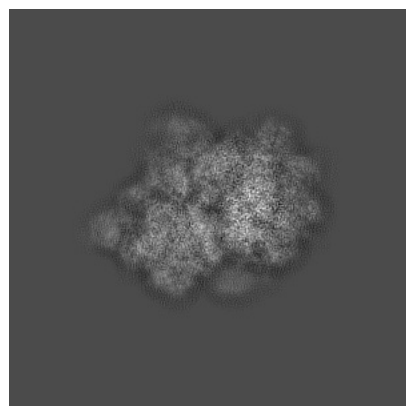
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11644. These allow visual inspection of the internal detail of the map and identification of artifacts.

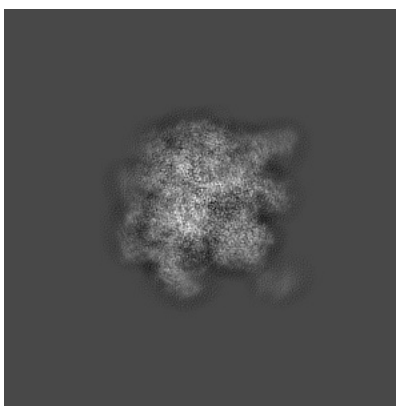
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

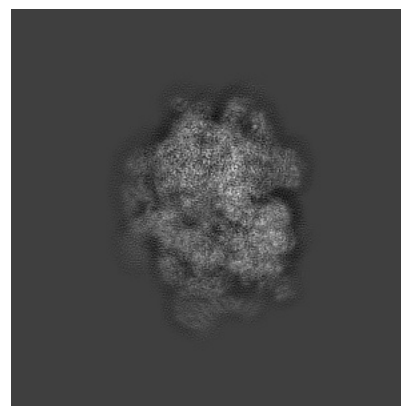
5.1.1 Primary map



X

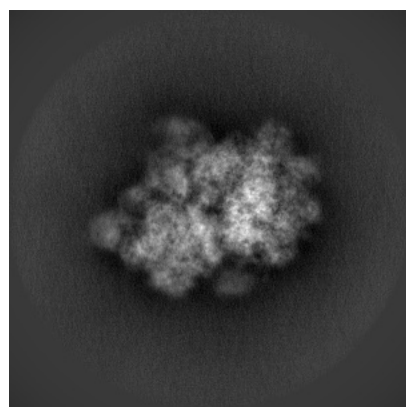


Y

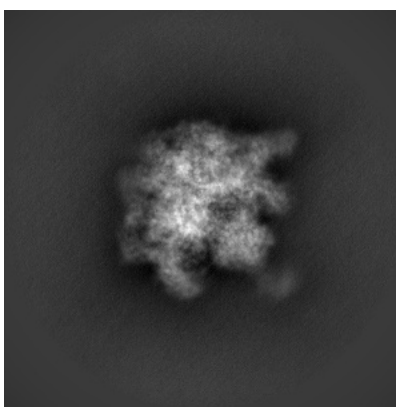


Z

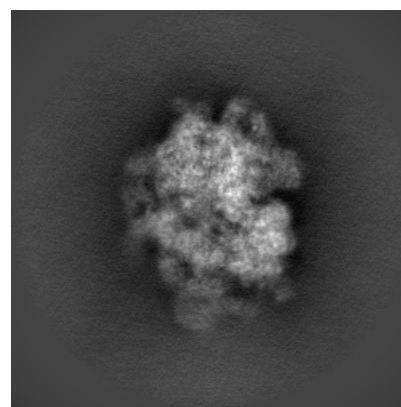
5.1.2 Raw map



X



Y

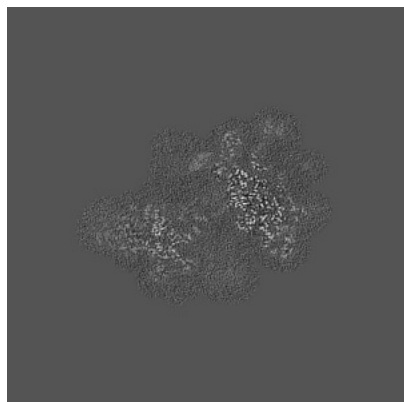


Z

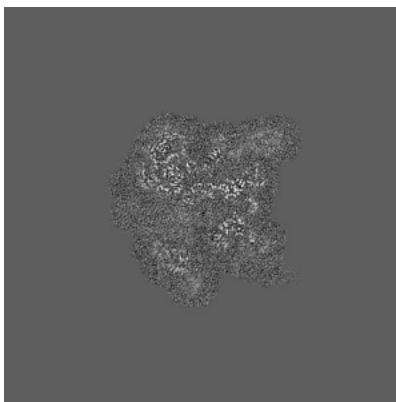
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

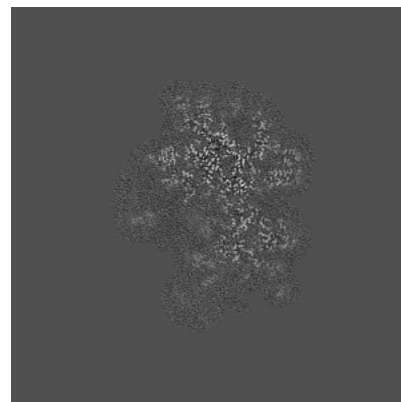
5.2.1 Primary map



X Index: 256

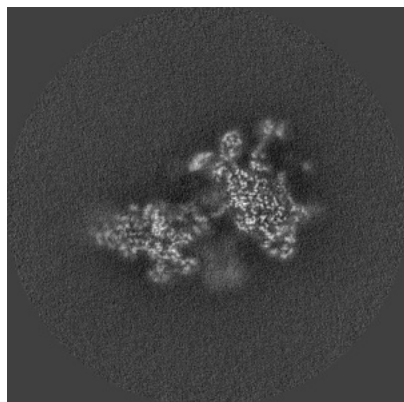


Y Index: 256

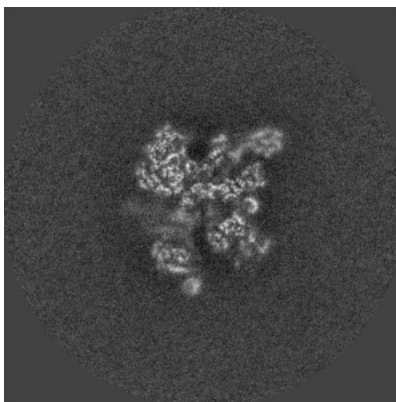


Z Index: 256

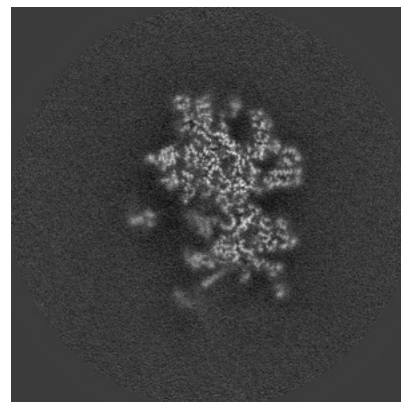
5.2.2 Raw map



X Index: 256



Y Index: 256

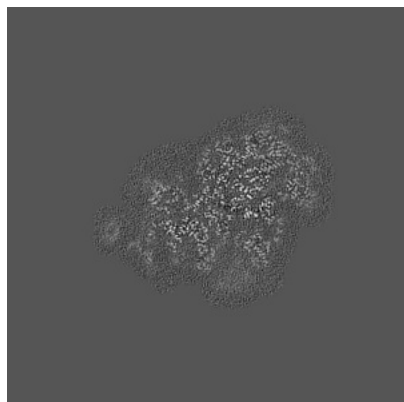


Z Index: 256

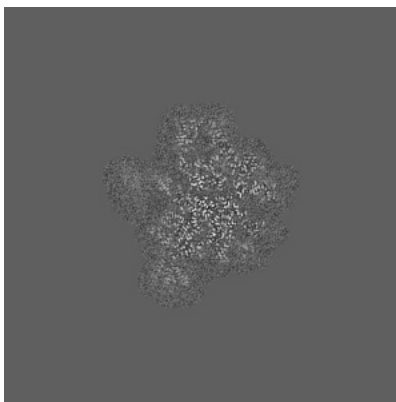
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

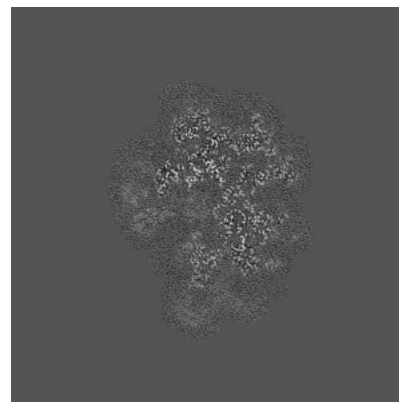
5.3.1 Primary map



X Index: 283

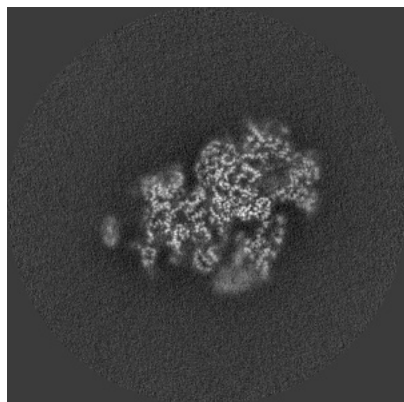


Y Index: 305

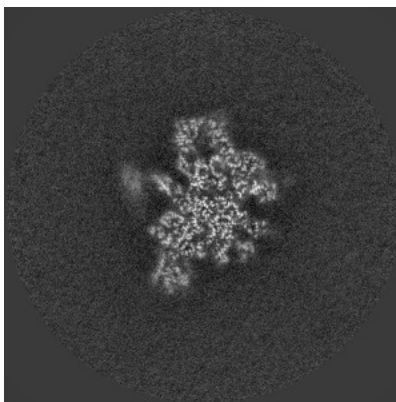


Z Index: 236

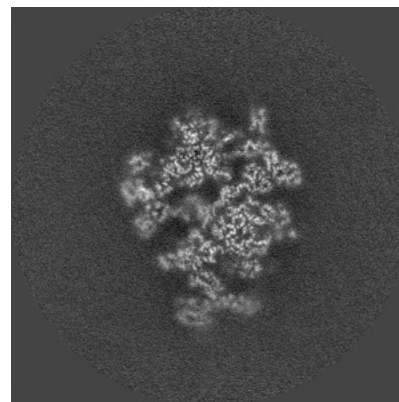
5.3.2 Raw map



X Index: 287



Y Index: 305

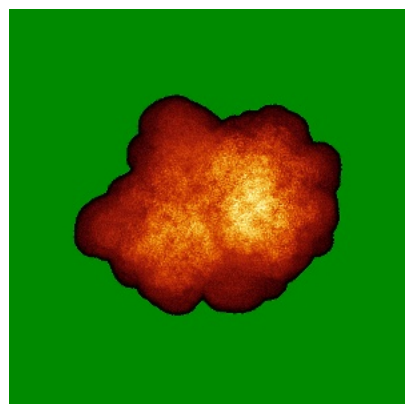


Z Index: 228

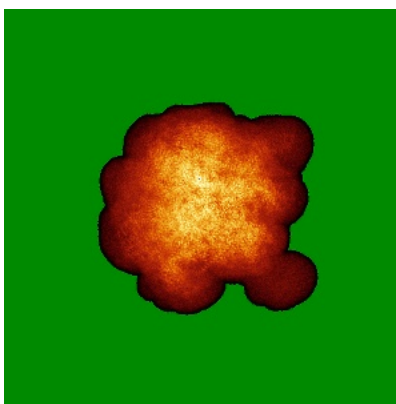
The images above show the largest variance slices of the map in three orthogonal directions.

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

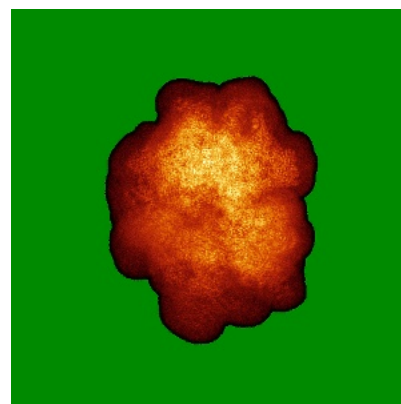
5.4.1 Primary map



X

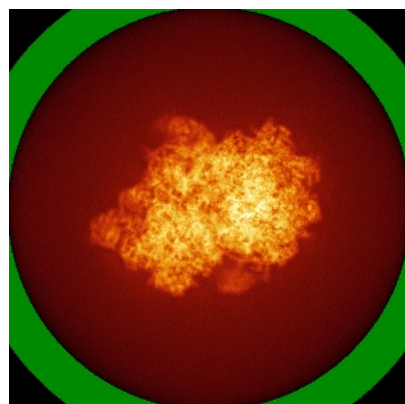


Y

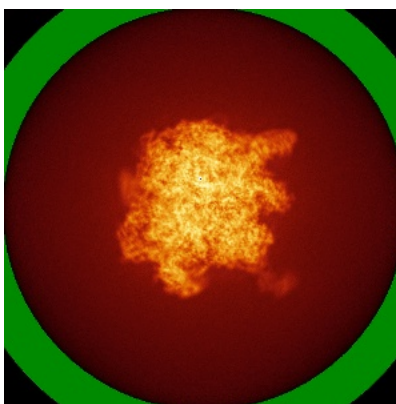


Z

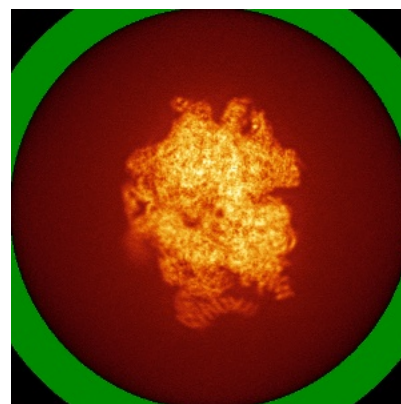
5.4.2 Raw map



X



Y

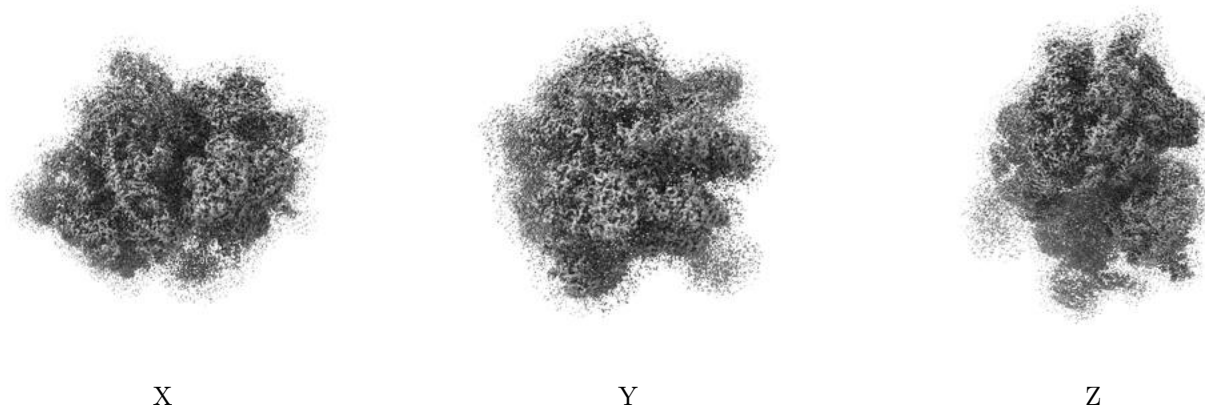


Z

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 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

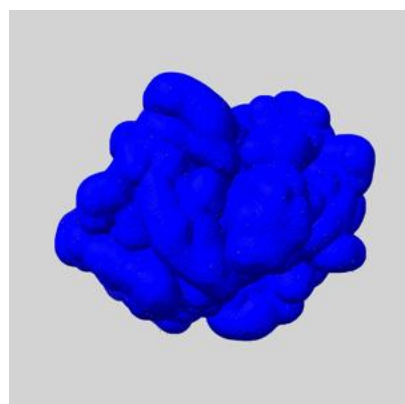
5.6 Mask visualisation [i](#)

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

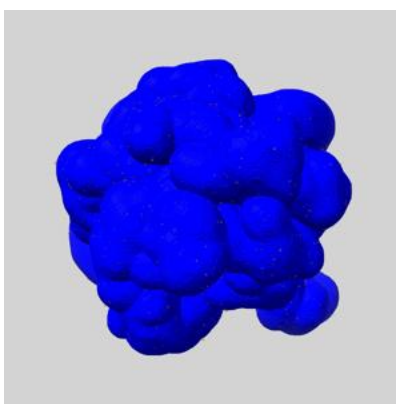
A mask typically either:

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

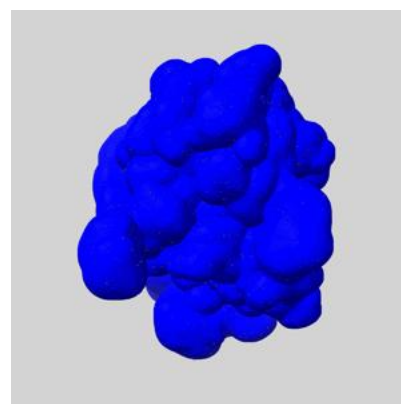
5.6.1 emd_11644_msk_1.map [i](#)



X



Y

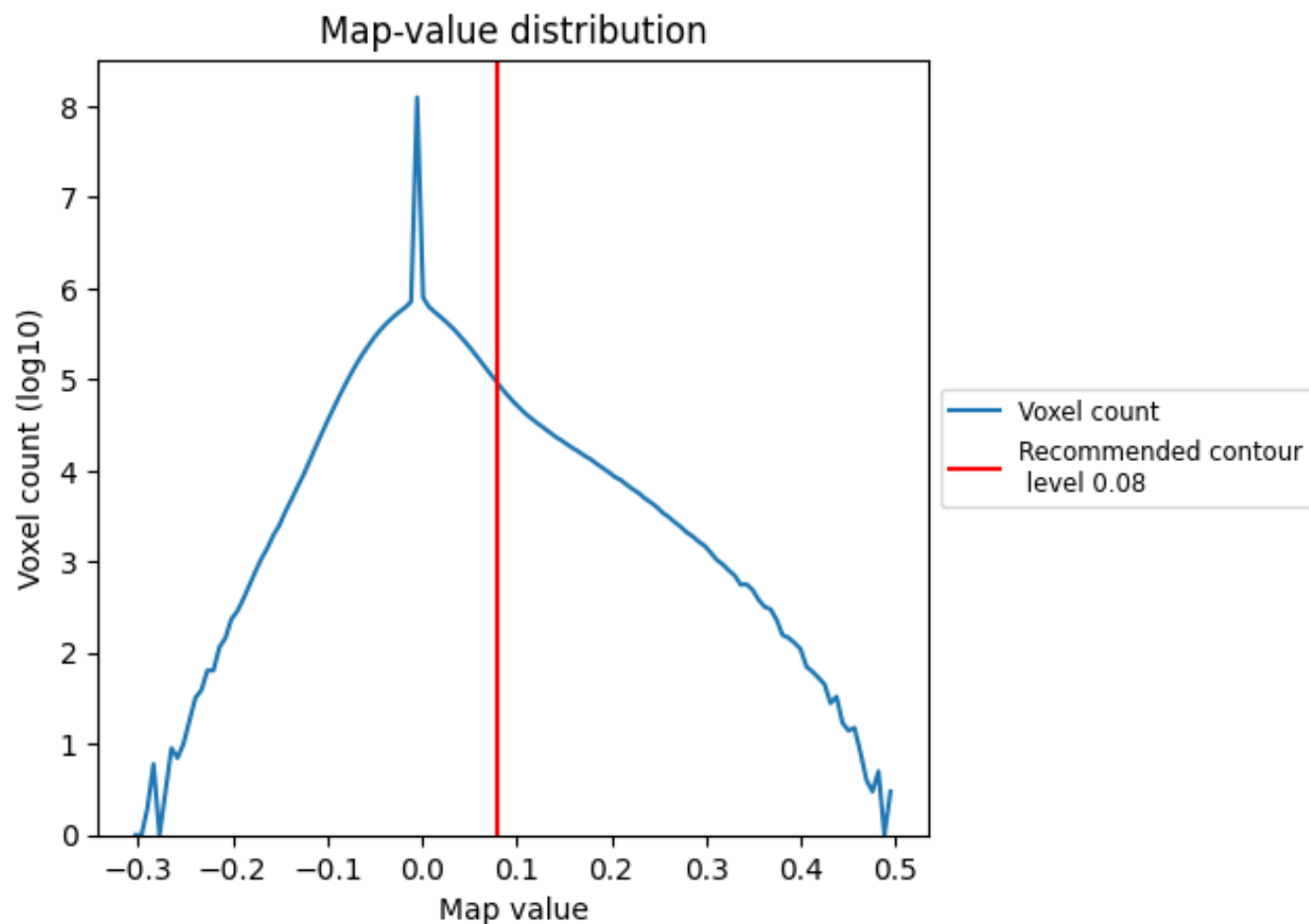


Z

6 Map analysis [i](#)

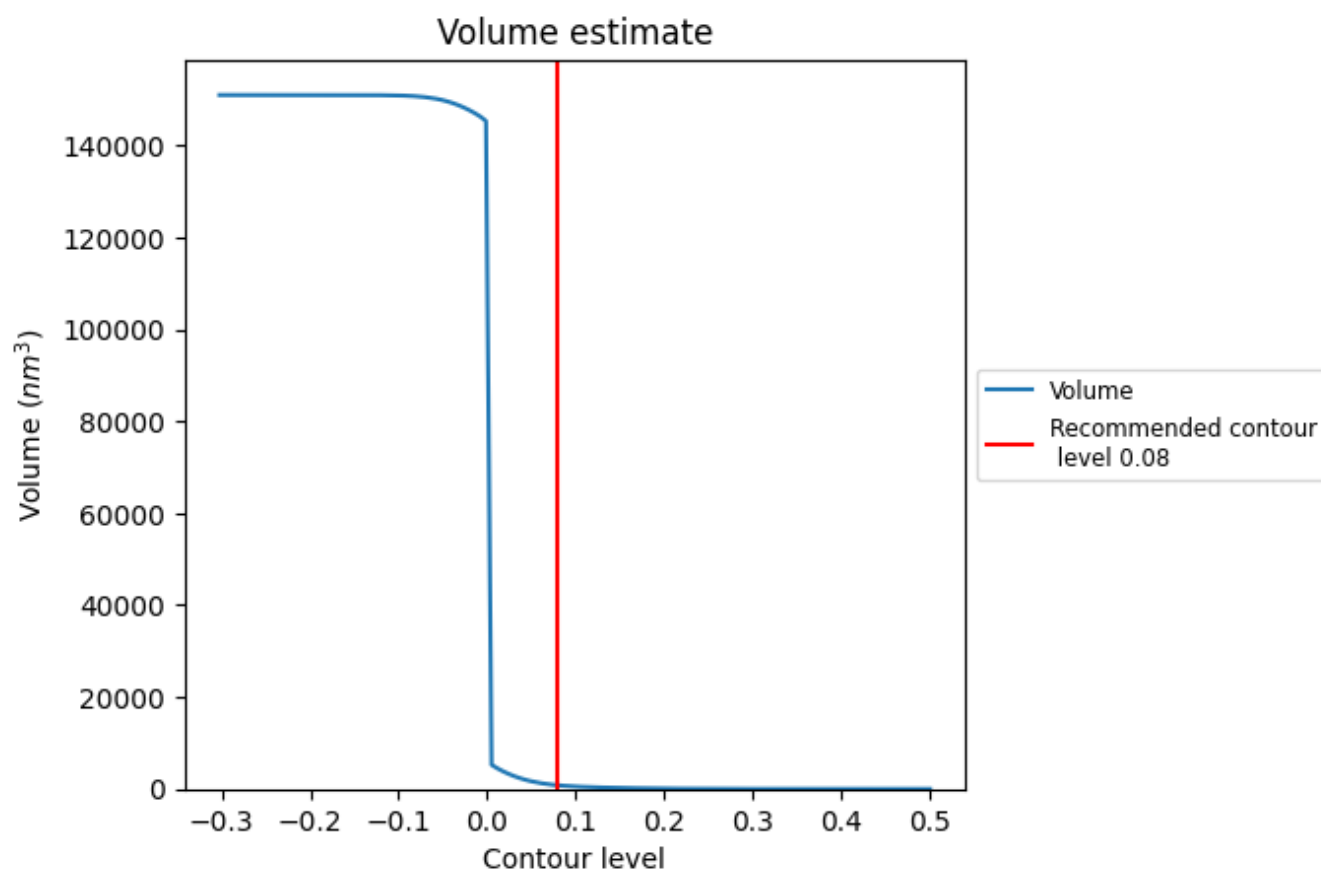
This section contains the results of statistical analysis of the map.

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.

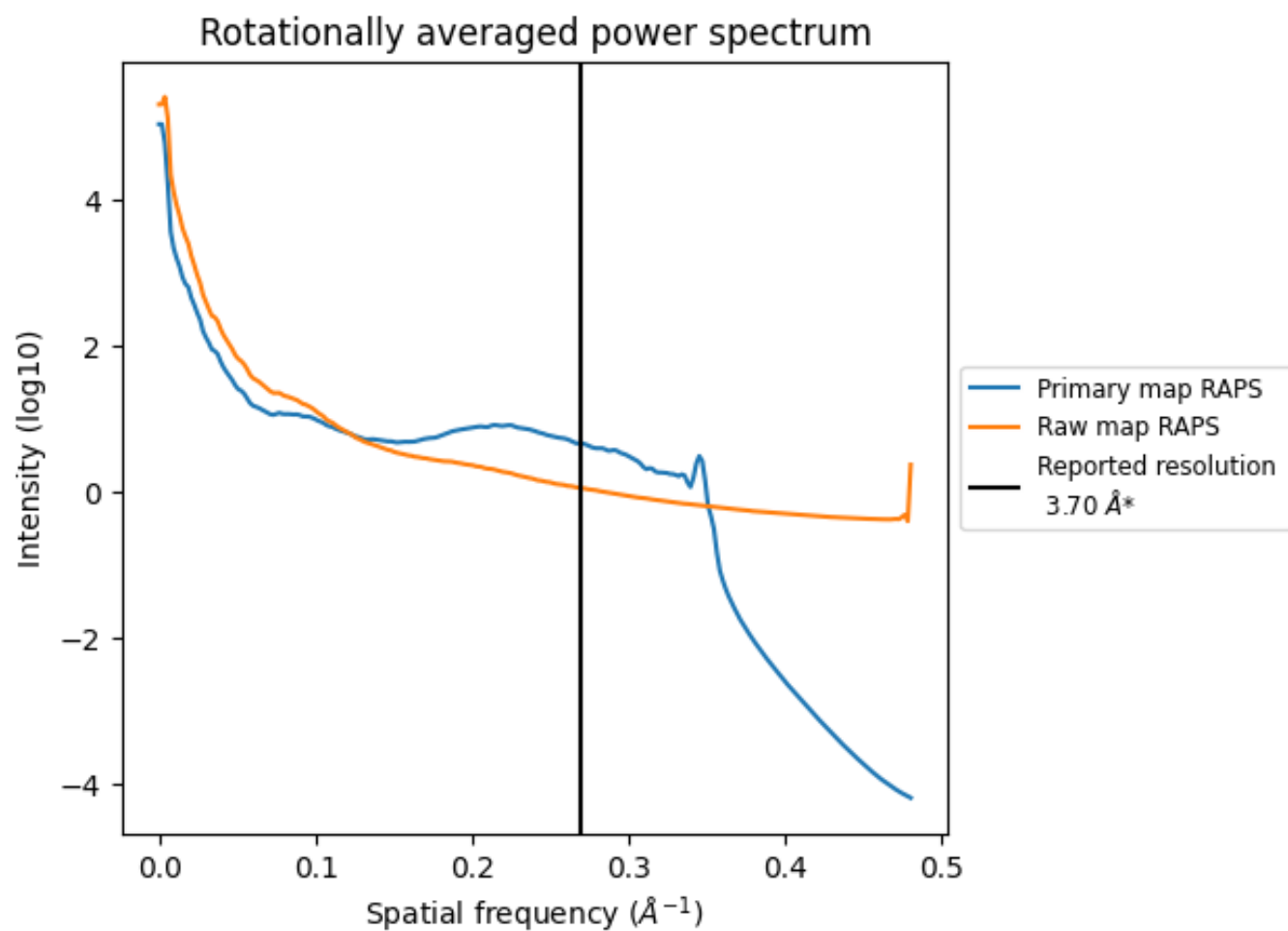
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 802 nm³; this corresponds to an approximate mass of 725 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 ⓘ

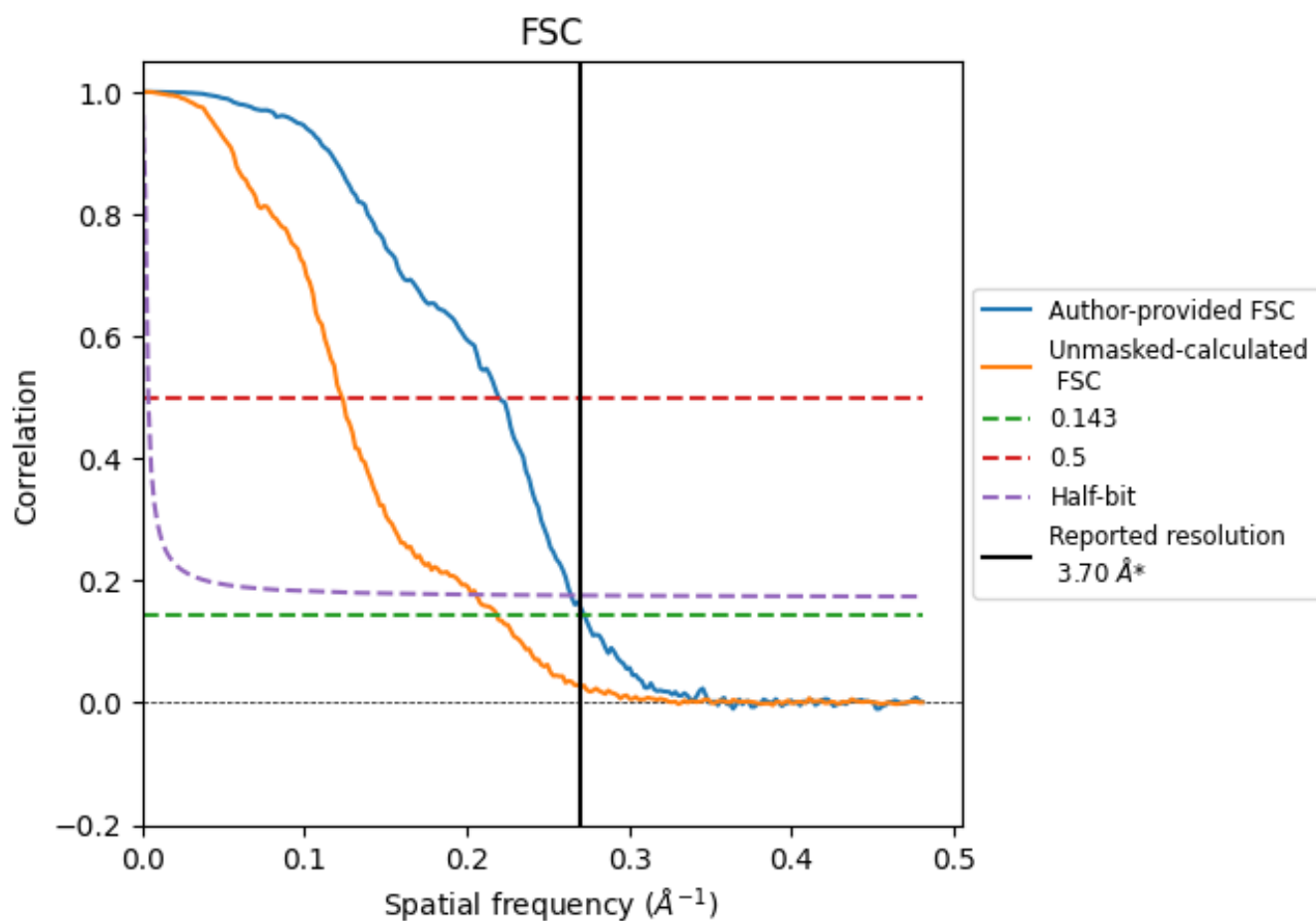


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 $\text{\AA}^{-1}$

7.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.67	4.55	3.78
Unmasked-calculated*	4.57	8.12	4.86

*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 4.57 differs from the reported value 3.7 by more than 10 %

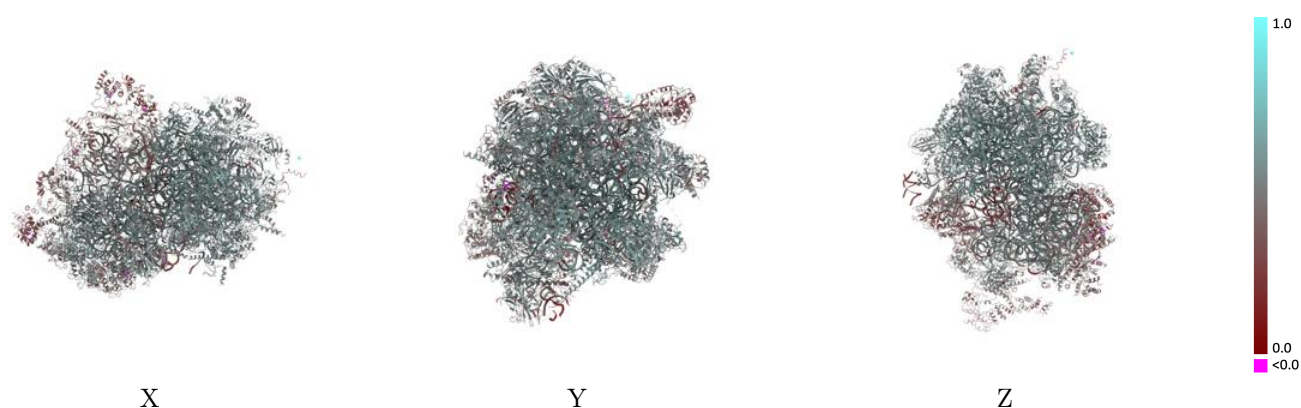
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11644 and PDB model 7A5I. Per-residue inclusion information can be found in section ?? on page ??.

8.1 Map-model overlay [i](#)

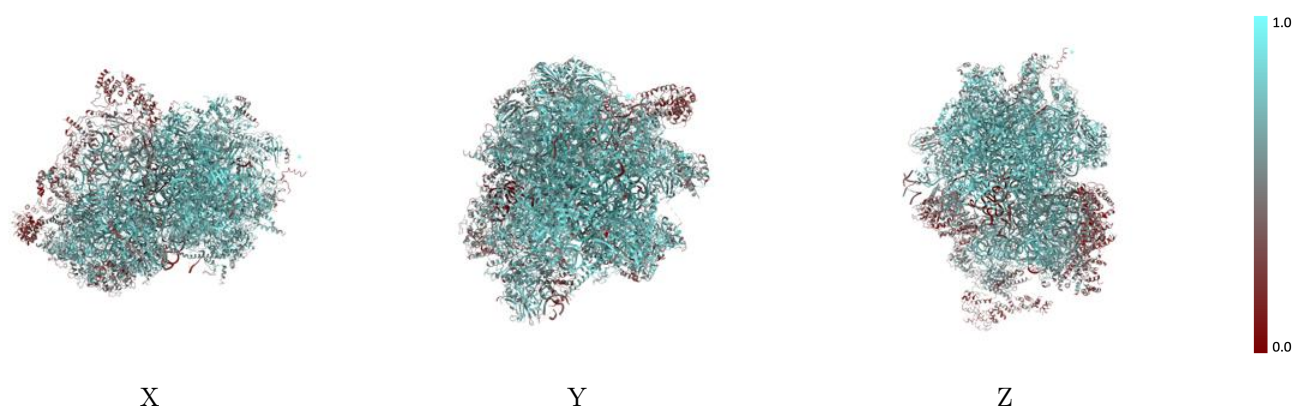
This section was not generated.

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



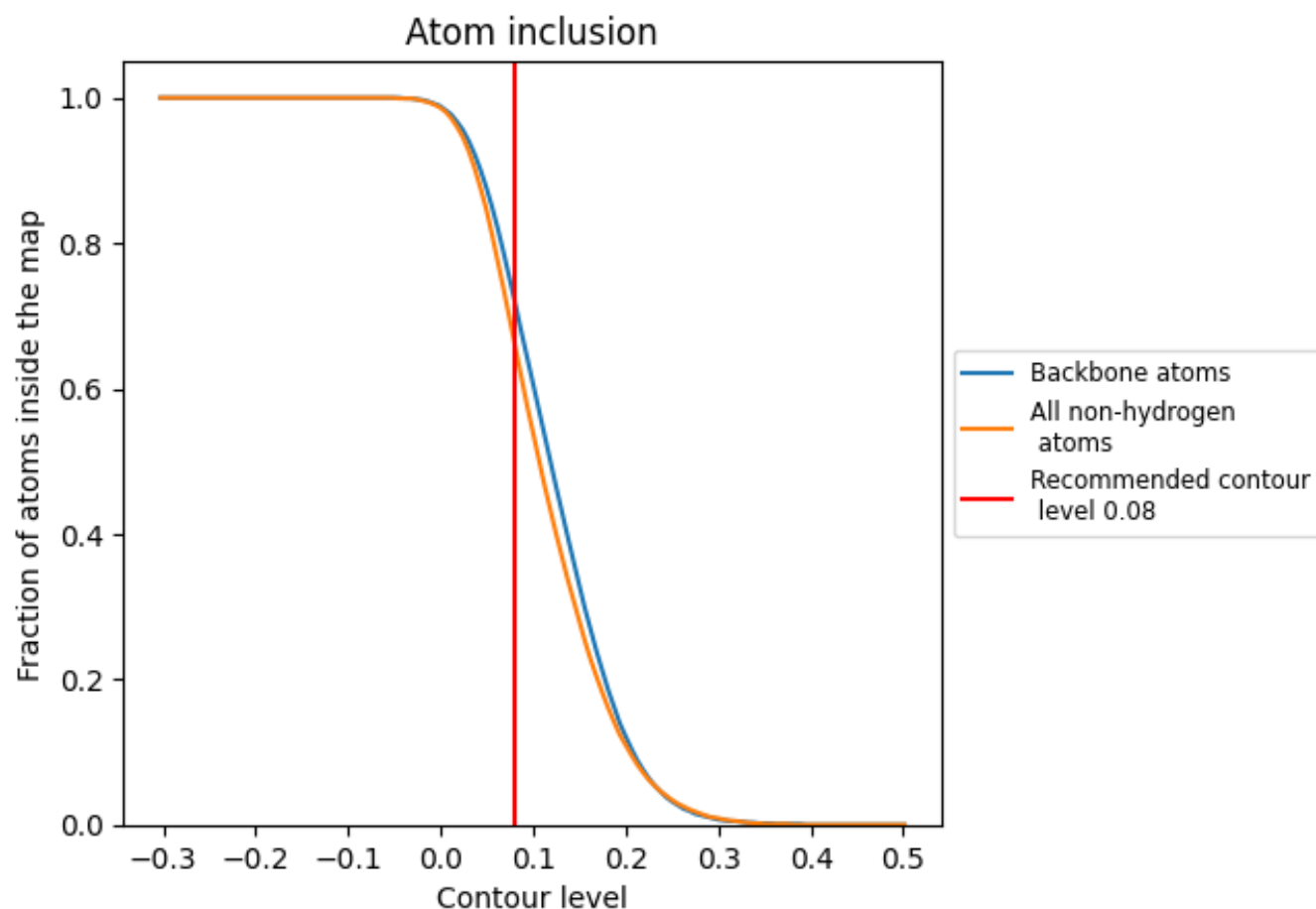
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

8.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 66% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6610	 0.4940
03	 0.6880	 0.5250
13	 0.7000	 0.5190
23	 0.8360	 0.5970
33	 0.8170	 0.5820
43	 0.8400	 0.5810
53	 0.7140	 0.5220
63	 0.6670	 0.4880
73	 0.6230	 0.4920
83	 0.4030	 0.3890
93	 0.7020	 0.5200
94	 0.3780	 0.3530
99	 0.0190	 0.1600
A3	 0.8330	 0.5430
A5	 0.0140	 0.2530
A6	 0.7720	 0.5010
B3	 0.6070	 0.3700
B6	 0.6880	 0.5130
C6	 0.6270	 0.5160
D3	 0.7450	 0.5560
D6	 0.5820	 0.4980
E3	 0.7510	 0.5480
E6	 0.6110	 0.5070
F3	 0.7670	 0.5480
F6	 0.5470	 0.4640
G6	 0.5520	 0.4720
H3	 0.6020	 0.5130
H6	 0.5950	 0.4820
I3	 0.4190	 0.4190
I6	 0.6520	 0.5120
J3	 0.2850	 0.3340
J6	 0.5740	 0.5070
K3	 0.7780	 0.5550
K6	 0.6560	 0.5010
L3	 0.6920	 0.5410



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Chain	Atom inclusion	Q-score
L6	 0.6220	 0.4990
M3	 0.7450	 0.5440
M6	 0.4660	 0.4300
N3	 0.7240	 0.5400
N6	 0.6570	 0.5060
O3	 0.7620	 0.5470
O6	 0.4680	 0.4300
P3	 0.7150	 0.5290
P6	 0.6580	 0.5130
Q3	 0.6800	 0.5320
Q6	 0.7060	 0.5300
R3	 0.7730	 0.5640
R6	 0.4040	 0.4110
S3	 0.7560	 0.5530
S6	 0.5420	 0.4580
T3	 0.7440	 0.5520
T6	 0.6170	 0.5010
U3	 0.7710	 0.5490
U6	 0.4820	 0.4330
V3	 0.5950	 0.4870
V6	 0.2470	 0.3250
W3	 0.7810	 0.5700
W6	 0.6260	 0.4970
X	 0.1410	 0.2620
X3	 0.6850	 0.5150
X6	 0.4690	 0.4200
Y2	 0.2280	 0.3150
Y3	 0.7510	 0.5450
Y6	 0.4450	 0.4310
Z3	 0.7730	 0.5590
Z6	 0.5470	 0.4690
a3	 0.7310	 0.5420
a6	 0.3740	 0.3940
b3	 0.7670	 0.5480
b6	 0.4690	 0.4250
c3	 0.6860	 0.5180
c6	 0.5050	 0.4700
d3	 0.6130	 0.4830
d6	 0.6670	 0.5380
e3	 0.3360	 0.3660
e6	 0.2900	 0.3500
f3	 0.5210	 0.4630

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g3	 0.7310	 0.5340
h3	 0.5790	 0.4620
i3	 0.8050	 0.5700
i4	 0.5510	 0.4430
j3	 0.6870	 0.5330
k3	 0.3990	 0.3730
l3	 0.6310	 0.4940
m3	 0.5750	 0.4800
o3	 0.7920	 0.5640
p3	 0.6100	 0.4900
q3	 0.5880	 0.4970
r3	 0.7520	 0.5380
s3	 0.7260	 0.5370
t3	 0.2860	 0.3230