



## wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 02:17 pm GMT

PDB ID : 8BH4  
EMDB ID : EMD-16047  
Title : Elongating E. coli 70S ribosome containing deacylated tRNA(iMet) in the P-site and AAm6A mRNA codon with cognate dipeptidyl-tRNA(Lys) in the A-site  
Authors : Koziej, L.; Glatt, S.  
Deposited on : 2022-10-29  
Resolution : 2.62 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

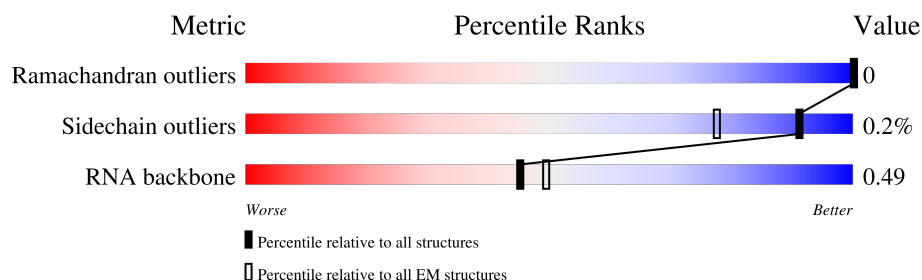
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 2.62 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.



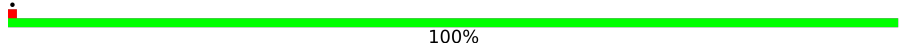
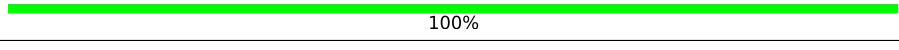
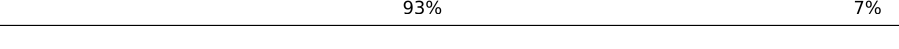
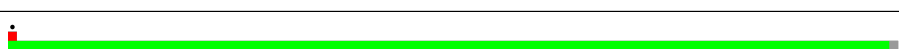
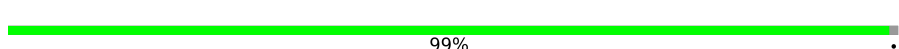
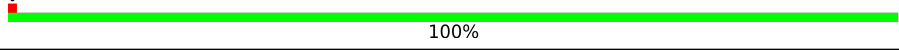
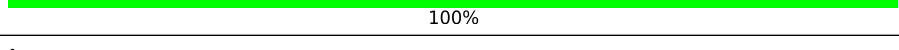
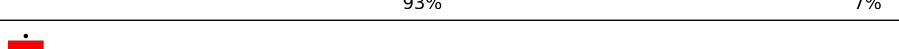


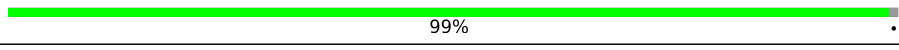
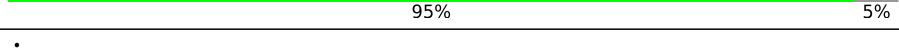
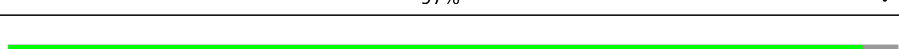
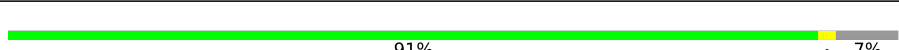
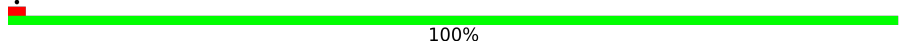
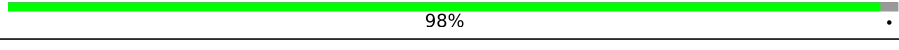
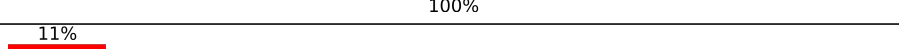

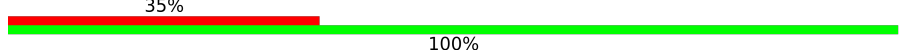
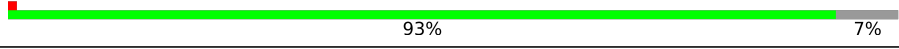




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	273	
2	B	209	
3	C	201	
4	D	179	
5	E	177	
6	F	149	
7	G	142	
8	H	123	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
9	I	144	
10	J	136	
11	K	127	
12	L	117	
13	M	115	
14	N	118	
15	O	103	
16	P	110	
17	Q	100	
18	R	104	
19	S	94	
20	T	85	
21	U	78	
22	V	63	
23	W	59	
24	a	57	
25	b	55	
26	c	46	
27	d	65	
28	e	38	
29	f	241	
30	g	233	
31	h	206	
32	i	167	
33	j	131	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	k	179	
35	l	130	
36	m	130	
37	n	103	
38	o	129	
39	p	124	
40	q	118	
41	r	101	
42	s	89	
43	t	82	
44	u	84	
45	v	75	
46	w	92	
47	x	87	
48	y	71	
49	0	2904	
50	1	120	
51	2	1542	
52	3	30	
53	4	77	
54	5	76	
55	6	2	

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 237726 atoms, of which 95530 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	208	Total	C	H	N	O	S	0	0
			3170	976	1611	287	292	4		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	177	Total	C	H	N	O	S	0	0
			2854	899	1444	249	256	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	173	Total	C	H	N	O	S	0	0
			2627	814	1332	237	242	2		

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	123	Total	C	H	N	O	S	0	0
			1970	593	1023	181	167	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 10 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	118	Total	C	H	N	O	S	0	0
			1934	585	989	194	161	5		

- Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	116	Total	C	H	N	O		0	0
			1815	552	923	178	162			

- Molecule 13 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 14 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	117	Total	C	H	N	O	0	0
			1966	604	1019	192	151		

- Molecule 15 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 16 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	93	Total	C	H	N	O	S	0	0
			1545	466	807	139	131	2		

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total	C	H	N	O	0	0
			1610	492	831	146	141		

- Molecule 19 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	75	Total	C	H	N	O	S	0	0
			1165	355	593	116	100	1		

- Molecule 21 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	60	Total	C	H	N	O	S	0	0
			1014	303	523	96	91	1		

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	57	Total	C	H	N	O	S	0	0
			921	276	482	86	75	2		

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	a	55	Total	C	H	N	O	S	0	0
			879	263	445	92	78	1		

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	b	51	Total	C	H	N	O	S	0	0
			868	269	451	76	72			

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	c	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	d	64	Total	C	H	N	O	S	0	0
			1077	323	573	105	74	2		

- Molecule 28 is a protein called 50S ribosomal protein L36.



Mol	Chain	Residues	Atoms						AltConf	Trace
28	e	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 29 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	f	224	Total	C	H	N	O	S	0	0
			3533	1109	1780	315	321	8		

- Molecule 30 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	g	206	Total	C	H	N	O	S	0	0
			3320	1028	1696	305	288	3		

- Molecule 31 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	h	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 32 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	i	155	Total	C	H	N	O	S	0	0
			2329	711	1185	216	211	6		

- Molecule 33 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	j	106	Total	C	H	N	O	S	0	0
			1726	545	864	156	154	7		

- Molecule 34 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	k	151	Total	C	H	N	O	S	0	0
			2419	735	1238	227	215	4		

- Molecule 35 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	l	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 36 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	m	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

- Molecule 37 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	n	99	Total	C	H	N	O	S	0	0
			1631	498	836	152	144	1		

- Molecule 38 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	o	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

- Molecule 39 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	p	123	Total	C	H	N	O	S	0	0
			1971	590	1016	196	165	4		

- Molecule 40 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	q	114	Total	C	H	N	O	S	0	0
			1824	546	941	178	156	3		

- Molecule 41 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	r	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 42 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	s	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 43 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	t	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 44 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	u	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 45 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	v	66	Total	C	H	N	O	S	0	0
			1109	345	565	102	96	1		

- Molecule 46 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	w	79	Total	C	H	N	O	S	0	0
			1302	408	665	120	107	2		

- Molecule 47 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	x	86	Total	C	H	N	O	S	0	0
			1389	414	719	138	115	3		

- Molecule 48 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	y	70	Total	C	H	N	O	S	0	0
			1219	366	629	125	98	1		

- Molecule 49 is a RNA chain called 23S rRNA RRLG-RRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	0	2758	Total	C	H	N	O	P	0	0
			89005	26417	29786	10911	19134	2757		

- Molecule 50 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	1	120	Total	C	H	N	O	P	0	0
			3868	1144	1302	468	835	119		

- Molecule 51 is a RNA chain called 16S rRNA RRSB-RRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	2	1534	Total	C	H	N	O	P	0	0
			49480	14681	16563	6041	10661	1534		

- Molecule 52 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	3	10	Total	C	H	N	O	P	0	0
			325	98	109	41	67	10		

- Molecule 53 is a RNA chain called Deacylated P-site tRNA(fMet).

Mol	Chain	Residues	Atoms							AltConf	Trace
53	4	77	Total	C	H	N	O	P	S	0	0
			2468	734	826	297	534	76	1		

- Molecule 54 is a RNA chain called Dipeptidyl A-site tRNA(Lys).

Mol	Chain	Residues	Atoms							AltConf	Trace
54	5	76	Total	C	H	N	O	P	S	0	0
			2456	729	831	283	537	75	1		

- Molecule 55 is a protein called fMet-Lys dipeptide.

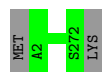
Mol	Chain	Residues	Atoms						AltConf	Trace
55	6	2	Total	C	H	N	O	S	0	0
			37	12	18	3	3	1		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 50S ribosomal protein L2

Chain A:  99%



- Molecule 2: 50S ribosomal protein L3

Chain B:  100%



- Molecule 3: 50S ribosomal protein L4

Chain C:  100%

There are no outlier residues recorded for this chain.

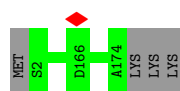
- Molecule 4: 50S ribosomal protein L5

Chain D:  8% 98% ..

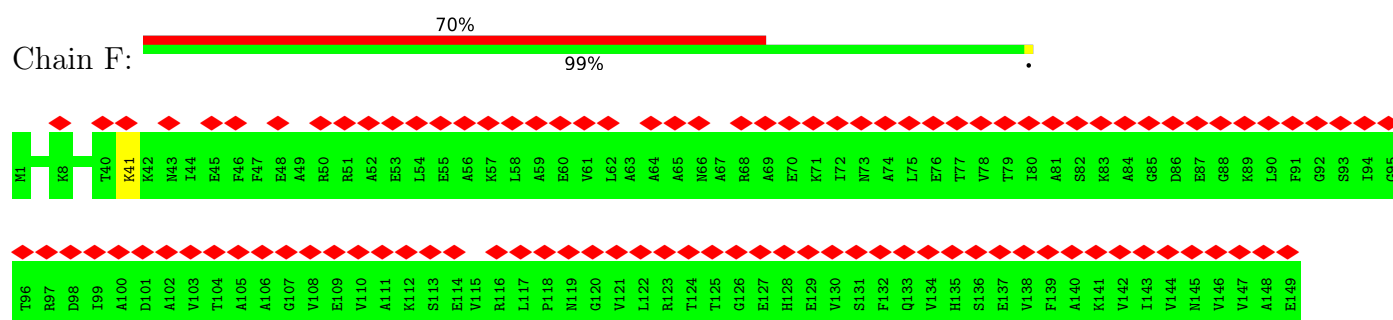


- Molecule 5: 50S ribosomal protein L6

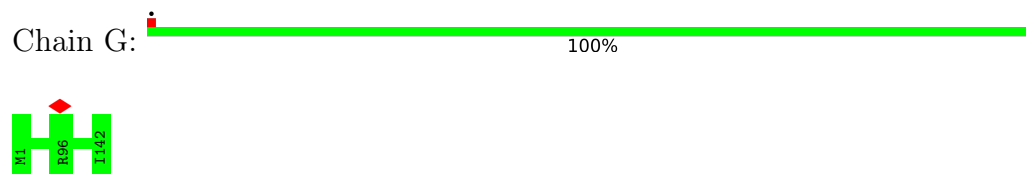
Chain E:  98%



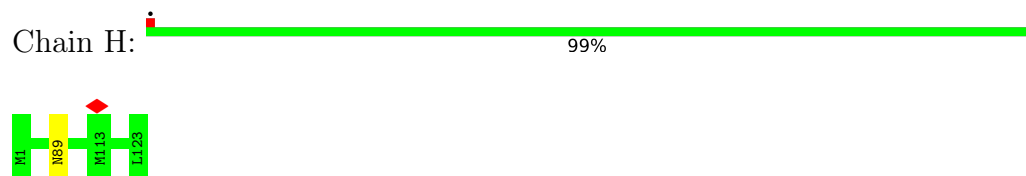
- Molecule 6: 50S ribosomal protein L9



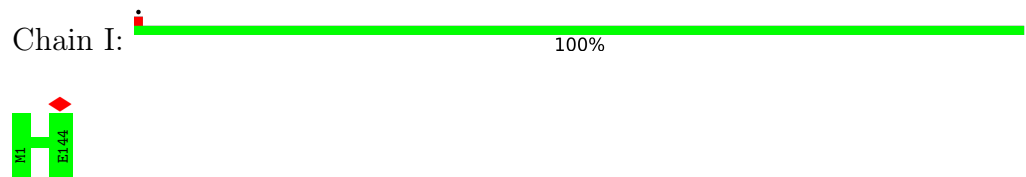
- Molecule 7: 50S ribosomal protein L13



- Molecule 8: 50S ribosomal protein L14



- Molecule 9: 50S ribosomal protein L15

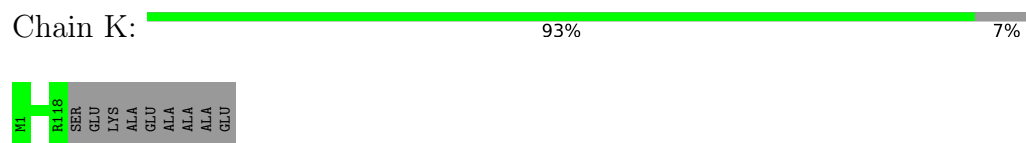


- Molecule 10: 50S ribosomal protein L16



There are no outlier residues recorded for this chain.

- Molecule 11: 50S ribosomal protein L17



- Molecule 12: 50S ribosomal protein L18





- Molecule 13: 50S ribosomal protein L19

Chain M: 99%



- Molecule 14: 50S ribosomal protein L20

Chain N: 99%



- Molecule 15: 50S ribosomal protein L21

Chain O: 100%



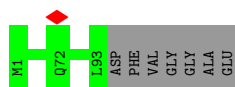
- Molecule 16: 50S ribosomal protein L22

Chain P: 100%



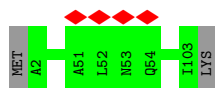
- Molecule 17: 50S ribosomal protein L23

Chain Q: 93% 7%



- Molecule 18: 50S ribosomal protein L24

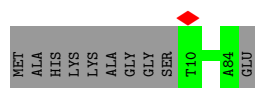
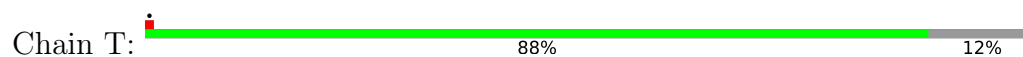
Chain R: 98%



- Molecule 19: 50S ribosomal protein L25



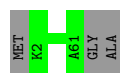
- Molecule 20: 50S ribosomal protein L27



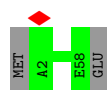
- Molecule 21: 50S ribosomal protein L28



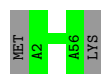
- Molecule 22: 50S ribosomal protein L29



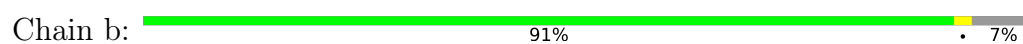
- Molecule 23: 50S ribosomal protein L30



- Molecule 24: 50S ribosomal protein L32



- Molecule 25: 50S ribosomal protein L33



- Molecule 26: 50S ribosomal protein L34



Chain c:  100%



- Molecule 27: 50S ribosomal protein L35

Chain d:  98%

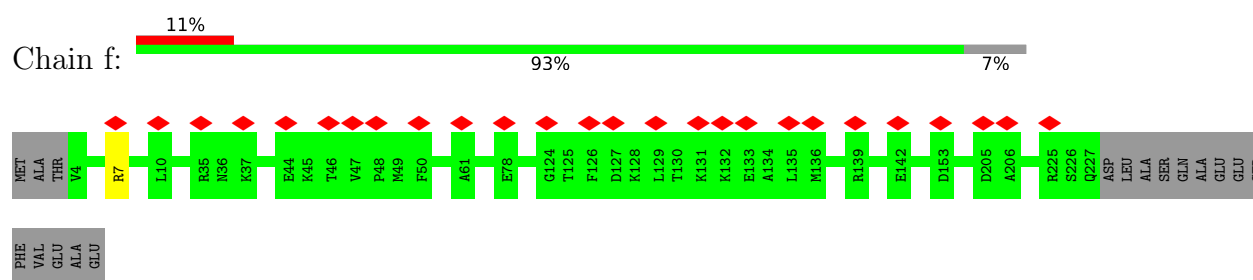


- Molecule 28: 50S ribosomal protein L36


Chain e:  100%

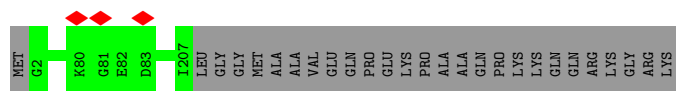
There are no outlier residues recorded for this chain.

- Molecule 29: 30S ribosomal protein S2



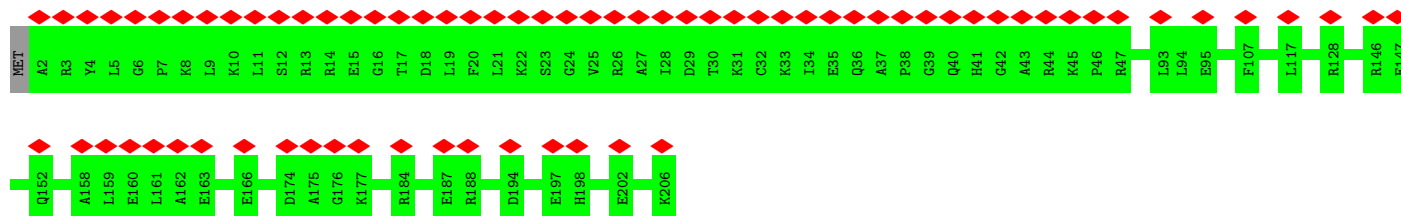
- Molecule 30: 30S ribosomal protein S3

Chain g:  88% 12%



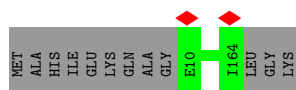
- Molecule 31: 30S ribosomal protein S4

Chain h:  35% 100%

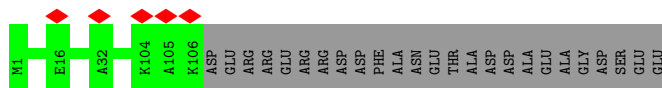
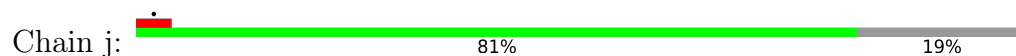


- Molecule 32: 30S ribosomal protein S5

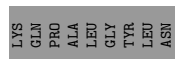
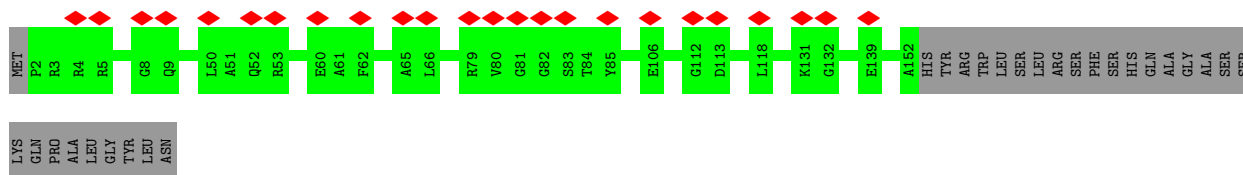
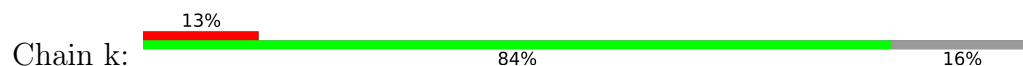
Chain i:  93% 7%



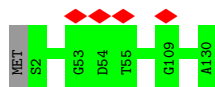
- Molecule 33: 30S ribosomal protein S6



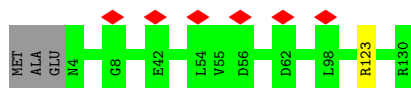
- Molecule 34: 30S ribosomal protein S7



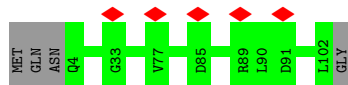
- Molecule 35: 30S ribosomal protein S8



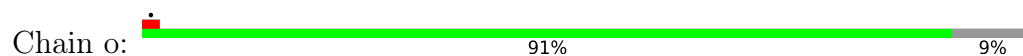
- Molecule 36: 30S ribosomal protein S9

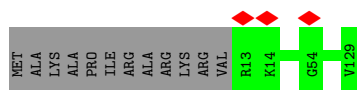


- Molecule 37: 30S ribosomal protein S10



- Molecule 38: 30S ribosomal protein S11

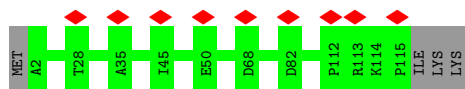




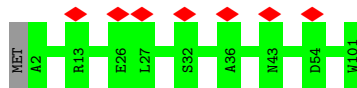
- Molecule 39: 30S ribosomal protein S12



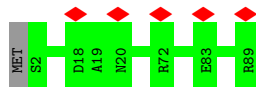
- Molecule 40: 30S ribosomal protein S13



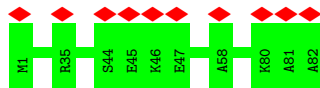
- Molecule 41: 30S ribosomal protein S14



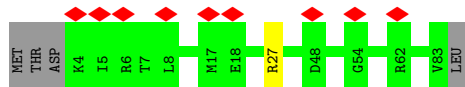
- Molecule 42: 30S ribosomal protein S15



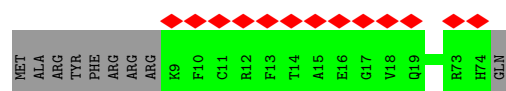
- Molecule 43: 30S ribosomal protein S16

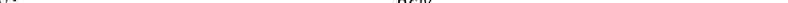


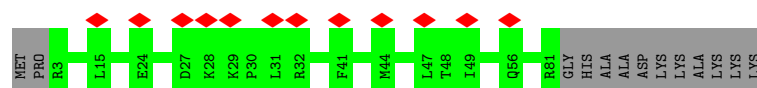
- Molecule 44: 30S ribosomal protein S17



- Molecule 45: 30S ribosomal protein S18



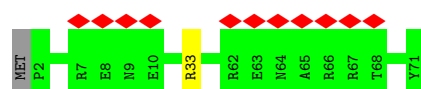
- Chain w: 

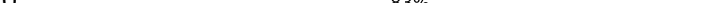


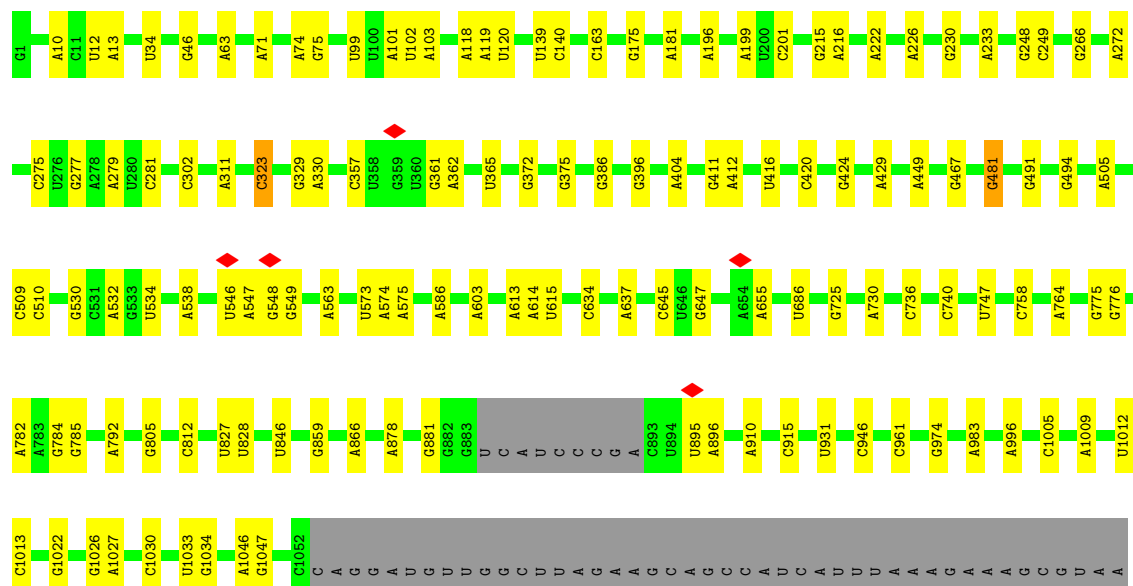
- Chain x: 



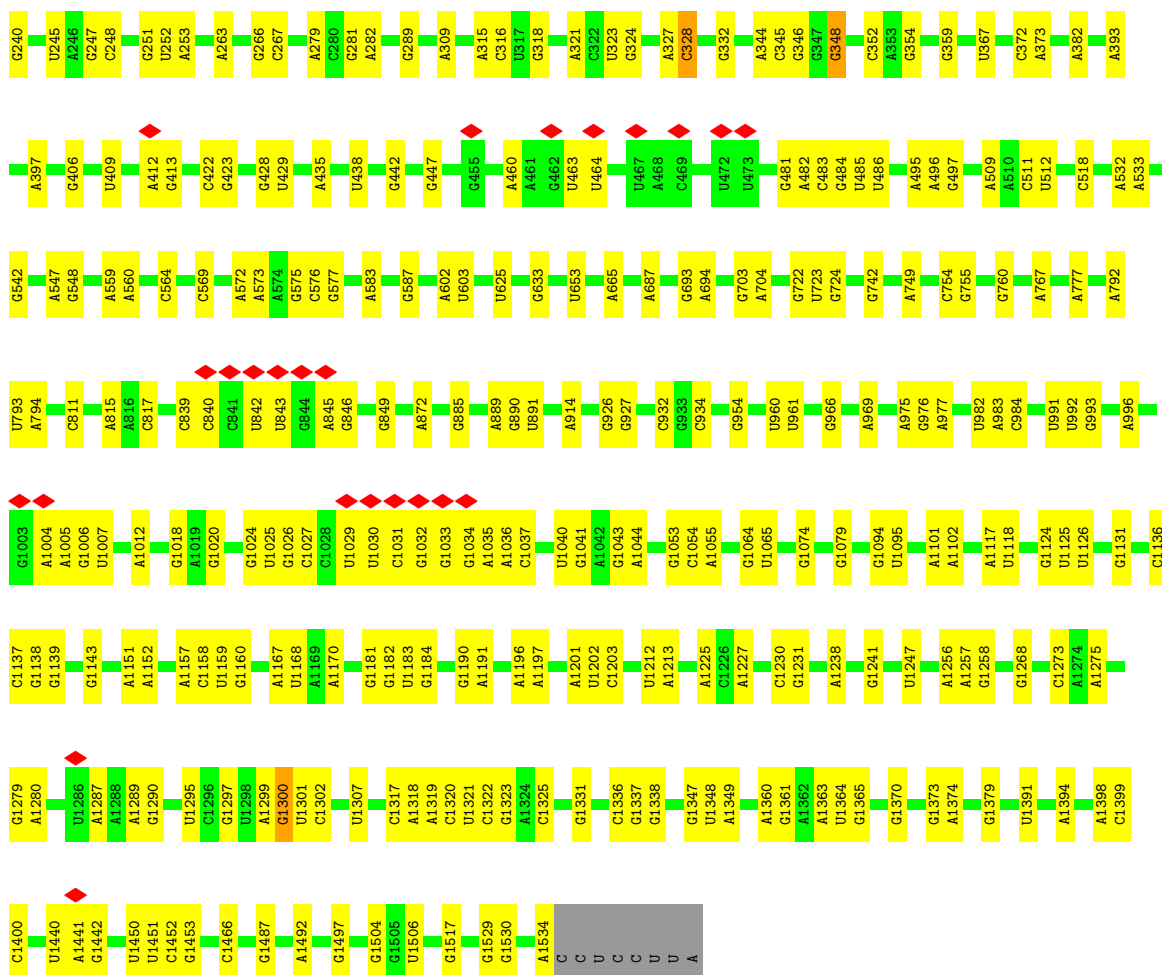
- Chain  $\gamma$ : 



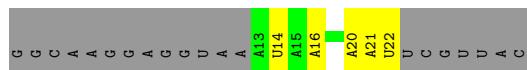
- Chain 0:  83% 12% 5%



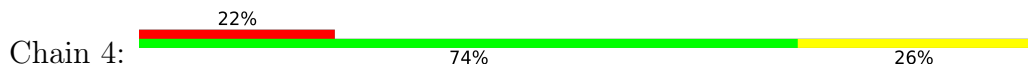




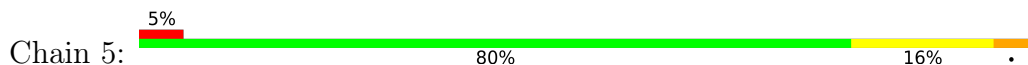
- Molecule 52: mRNA



- Molecule 53: Deacylated P-site tRNA(fMet)



- Molecule 54: Dipeptidyl A-site tRNA(Lys)



- Molecule 55: fMet-Lys dipeptide

Chain 6: 



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	271987	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.418	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.089	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: T6A, 4SU, 6MZ, U8U, OMC, H2U, FME, 5MU

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	0.32	0/2121	0.61	0/2852
2	B	0.29	0/1580	0.55	0/2127
3	C	0.29	0/1571	0.53	0/2113
4	D	0.27	0/1434	0.53	0/1926
5	E	0.30	0/1315	0.52	0/1783
6	F	0.25	0/1122	0.50	0/1515
7	G	0.32	0/1152	0.53	0/1551
8	H	0.29	0/956	0.59	0/1279
9	I	0.30	0/1062	0.60	0/1413
10	J	0.31	0/1093	0.61	0/1460
11	K	0.30	0/958	0.62	0/1281
12	L	0.31	0/902	0.57	0/1209
13	M	0.31	0/929	0.59	0/1242
14	N	0.33	0/960	0.58	0/1278
15	O	0.32	0/829	0.57	0/1107
16	P	0.28	0/864	0.57	0/1156
17	Q	0.29	0/744	0.54	0/994
18	R	0.29	0/787	0.52	0/1051
19	S	0.30	0/766	0.52	0/1025
20	T	0.29	0/579	0.57	0/767
21	U	0.28	0/635	0.61	0/848
22	V	0.28	0/492	0.54	0/655
23	W	0.28	0/443	0.57	0/593
24	a	0.28	0/440	0.60	0/588
25	b	0.27	0/424	0.52	0/565
26	c	0.30	0/380	0.68	0/498
27	d	0.28	0/513	0.60	0/676
28	e	0.31	0/303	0.60	0/397
29	f	0.26	0/1784	0.49	0/2403
30	g	0.29	0/1651	0.54	0/2225
31	h	0.28	0/1665	0.57	0/2227
32	i	0.28	0/1157	0.53	0/1557

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	j	0.27	0/881	0.52	0/1189
34	k	0.27	0/1195	0.55	0/1602
35	l	0.29	0/989	0.54	0/1326
36	m	0.28	0/1034	0.62	0/1375
37	n	0.27	0/805	0.59	0/1089
38	o	0.28	0/893	0.58	0/1205
39	p	0.29	0/969	0.61	0/1300
40	q	0.25	0/892	0.59	0/1193
41	r	0.28	0/817	0.58	0/1088
42	s	0.27	0/722	0.56	0/964
43	t	0.26	0/659	0.56	0/884
44	u	0.26	0/657	0.56	0/881
45	v	0.29	0/553	0.55	0/742
46	w	0.26	0/652	0.53	0/877
47	x	0.29	0/676	0.55	0/895
48	y	0.28	0/598	0.61	0/792
49	0	0.51	0/66326	0.84	7/103471 (0.0%)
50	1	0.45	0/2869	0.80	0/4474
51	2	0.46	0/36859	0.83	7/57501 (0.0%)
52	3	0.92	0/215	0.86	0/330
53	4	0.60	0/1766	0.73	0/2753
54	5	0.72	0/1663	0.74	0/2588
55	6	0.16	0/8	0.34	0/8
All	All	0.44	0/154309	0.77	14/230888 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	2	328	C	C2-N1-C1'	6.38	125.82	118.80
49	0	1313	U	C2-N1-C1'	6.01	124.92	117.70
49	0	2501	C	C6-N1-C2	-5.64	118.04	120.30
49	0	2321	U	C2-N1-C1'	5.54	124.35	117.70
51	2	1466	C	N3-C2-O2	-5.47	118.07	121.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	269/273 (98%)	251 (93%)	18 (7%)	0	100	100
2	B	206/209 (99%)	194 (94%)	12 (6%)	0	100	100
3	C	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
4	D	175/179 (98%)	159 (91%)	16 (9%)	0	100	100
5	E	171/177 (97%)	162 (95%)	9 (5%)	0	100	100
6	F	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
7	G	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
8	H	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
9	I	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
10	J	134/136 (98%)	120 (90%)	14 (10%)	0	100	100
11	K	116/127 (91%)	106 (91%)	10 (9%)	0	100	100
12	L	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
13	M	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
14	N	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
15	O	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
16	P	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
17	Q	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
18	R	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
19	S	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
20	T	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
21	U	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
22	V	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
23	W	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
24	a	53/57 (93%)	50 (94%)	3 (6%)	0	100	100
25	b	49/55 (89%)	47 (96%)	2 (4%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	c	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
27	d	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
28	e	36/38 (95%)	36 (100%)	0	0	100	100
29	f	222/241 (92%)	198 (89%)	24 (11%)	0	100	100
30	g	204/233 (88%)	189 (93%)	15 (7%)	0	100	100
31	h	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
32	i	153/167 (92%)	141 (92%)	12 (8%)	0	100	100
33	j	104/131 (79%)	98 (94%)	6 (6%)	0	100	100
34	k	149/179 (83%)	138 (93%)	11 (7%)	0	100	100
35	l	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
36	m	125/130 (96%)	112 (90%)	13 (10%)	0	100	100
37	n	97/103 (94%)	90 (93%)	7 (7%)	0	100	100
38	o	115/129 (89%)	108 (94%)	7 (6%)	0	100	100
39	p	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
40	q	112/118 (95%)	98 (88%)	14 (12%)	0	100	100
41	r	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
42	s	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
43	t	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
44	u	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
45	v	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
46	w	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
47	x	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
48	y	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	5525/5839 (95%)	5198 (94%)	327 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	216/218 (99%)	216 (100%)	0	100	100
2	B	164/164 (100%)	164 (100%)	0	100	100
3	C	165/165 (100%)	165 (100%)	0	100	100
4	D	148/150 (99%)	147 (99%)	1 (1%)	81	92
5	E	134/138 (97%)	134 (100%)	0	100	100
6	F	114/114 (100%)	113 (99%)	1 (1%)	75	89
7	G	116/116 (100%)	116 (100%)	0	100	100
8	H	104/104 (100%)	103 (99%)	1 (1%)	73	87
9	I	103/103 (100%)	103 (100%)	0	100	100
10	J	109/109 (100%)	109 (100%)	0	100	100
11	K	98/103 (95%)	98 (100%)	0	100	100
12	L	86/87 (99%)	86 (100%)	0	100	100
13	M	99/100 (99%)	99 (100%)	0	100	100
14	N	89/90 (99%)	89 (100%)	0	100	100
15	O	84/84 (100%)	84 (100%)	0	100	100
16	P	93/93 (100%)	93 (100%)	0	100	100
17	Q	80/84 (95%)	80 (100%)	0	100	100
18	R	83/85 (98%)	83 (100%)	0	100	100
19	S	78/78 (100%)	77 (99%)	1 (1%)	65	83
20	T	57/63 (90%)	57 (100%)	0	100	100
21	U	67/68 (98%)	67 (100%)	0	100	100
22	V	54/55 (98%)	54 (100%)	0	100	100
23	W	47/49 (96%)	47 (100%)	0	100	100
24	a	46/48 (96%)	46 (100%)	0	100	100
25	b	46/49 (94%)	45 (98%)	1 (2%)	47	70
26	c	38/38 (100%)	38 (100%)	0	100	100
27	d	51/52 (98%)	51 (100%)	0	100	100
28	e	34/34 (100%)	34 (100%)	0	100	100
29	f	186/199 (94%)	185 (100%)	1 (0%)	86	95
30	g	170/190 (90%)	170 (100%)	0	100	100
31	h	172/173 (99%)	172 (100%)	0	100	100
32	i	118/126 (94%)	118 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	j	92/112 (82%)	92 (100%)	0	100	100
34	k	124/147 (84%)	124 (100%)	0	100	100
35	l	104/105 (99%)	104 (100%)	0	100	100
36	m	105/107 (98%)	104 (99%)	1 (1%)	73	87
37	n	87/90 (97%)	87 (100%)	0	100	100
38	o	90/99 (91%)	90 (100%)	0	100	100
39	p	103/104 (99%)	103 (100%)	0	100	100
40	q	92/96 (96%)	92 (100%)	0	100	100
41	r	83/84 (99%)	83 (100%)	0	100	100
42	s	76/77 (99%)	76 (100%)	0	100	100
43	t	65/65 (100%)	65 (100%)	0	100	100
44	u	74/78 (95%)	73 (99%)	1 (1%)	62	81
45	v	57/65 (88%)	57 (100%)	0	100	100
46	w	70/79 (89%)	70 (100%)	0	100	100
47	x	65/66 (98%)	65 (100%)	0	100	100
48	y	60/61 (98%)	59 (98%)	1 (2%)	56	77
55	6	1/1 (100%)	1 (100%)	0	100	100
All	All	4597/4765 (96%)	4588 (100%)	9 (0%)	91	98

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	u	27	ARG
48	y	33	ARG
19	S	24	ASN
25	b	28	ARG
29	f	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
38	o	24	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	0	2754/2904 (94%)	348 (12%)	6 (0%)
50	1	119/120 (99%)	11 (9%)	0
51	2	1534/1542 (99%)	304 (19%)	53 (3%)
52	3	8/30 (26%)	4 (50%)	0
53	4	76/77 (98%)	16 (21%)	1 (1%)
54	5	74/76 (97%)	10 (13%)	2 (2%)
All	All	4565/4749 (96%)	693 (15%)	62 (1%)

5 of 693 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
49	0	10	A
49	0	12	U
49	0	13	A
49	0	34	U
49	0	46	G

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	2	842	U
51	2	1399	C
51	2	1031	C
51	2	1364	U
53	4	10	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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
53	4SU	4	7	53	18,21,22	1.82	4 (22%)	26,30,33	2.33	5 (19%)
55	FME	6	1	55	8,9,10	0.96	0	7,9,11	1.18	1 (14%)
54	H2U	5	20	54	18,21,22	0.97	2 (11%)	21,30,33	1.37	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	H2U	5	17	54	18,21,22	0.96	2 (11%)	21,30,33	1.37	3 (14%)
54	T6A	5	37	54	27,34,35	0.90	0	29,49,52	2.67	7 (24%)
54	U8U	5	34	54,52	19,24,25	1.62	3 (15%)	23,34,37	1.09	2 (8%)
54	5MU	5	54	54	19,22,23	1.40	4 (21%)	28,32,35	2.24	6 (21%)
53	5MU	4	54	53	19,22,23	1.38	6 (31%)	28,32,35	2.06	6 (21%)
52	6MZ	3	21	54,52	18,25,26	1.80	4 (22%)	16,36,39	2.24	4 (25%)
54	H2U	5	16	54	18,21,22	0.97	2 (11%)	21,30,33	1.36	3 (14%)
53	OMC	4	32	53	19,22,23	0.87	2 (10%)	26,31,34	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	4SU	4	7	53	-	1/7/25/26	0/2/2/2
55	FME	6	1	55	-	5/7/9/11	-
54	H2U	5	20	54	-	3/7/38/39	0/2/2/2
54	H2U	5	17	54	-	3/7/38/39	0/2/2/2
54	T6A	5	37	54	-	6/19/41/42	0/3/3/3
54	U8U	5	34	54,52	-	0/9/28/29	0/2/2/2
54	5MU	5	54	54	-	0/7/25/26	0/2/2/2
53	5MU	4	54	53	-	0/7/25/26	0/2/2/2
52	6MZ	3	21	54,52	-	2/5/27/28	0/3/3/3
54	H2U	5	16	54	-	1/7/38/39	0/2/2/2
53	OMC	4	32	53	-	0/9/27/28	0/2/2/2

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	3	21	6MZ	C6-N6	5.12	1.43	1.35
54	5	34	U8U	C2-S2	-5.05	1.59	1.67
53	4	7	4SU	C4-S4	-4.75	1.59	1.68
53	4	7	4SU	C4-N3	-3.66	1.33	1.37
54	5	34	U8U	C4-N3	-3.10	1.33	1.38

The worst 5 of 40 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
54	5	37	T6A	N6-C10-N11	8.21	125.22	113.76
53	4	7	4SU	C4-N3-C2	-7.22	120.32	127.34
54	5	37	T6A	C2-N1-C6	6.83	122.45	116.59
53	4	7	4SU	C5-C4-N3	5.98	120.24	114.69
52	3	21	6MZ	N3-C2-N1	-5.92	119.42	128.68

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	5	17	H2U	O4'-C1'-N1-C2
54	5	17	H2U	O4'-C1'-N1-C6
54	5	20	H2U	O4'-C1'-N1-C2
54	5	20	H2U	O4'-C1'-N1-C6
54	5	37	T6A	N11-C12-C14-O14

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

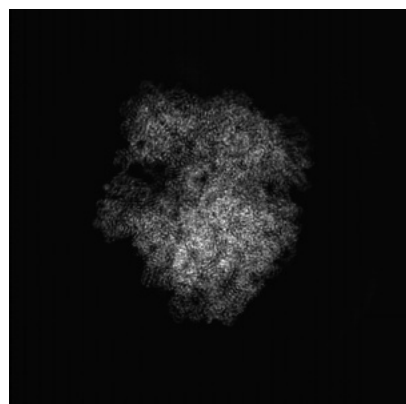
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16047. These allow visual inspection of the internal detail of the map and identification of artifacts.

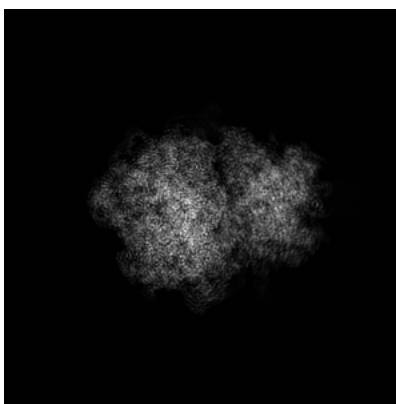
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

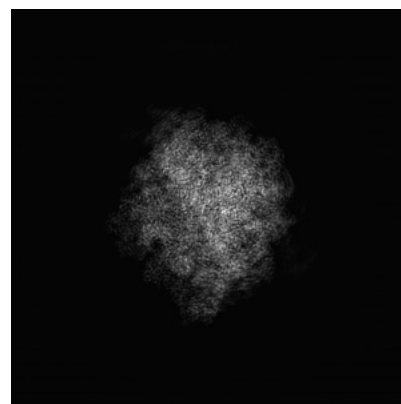
#### 6.1.1 Primary map



X

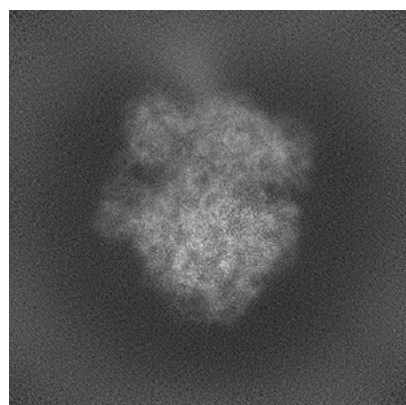


Y

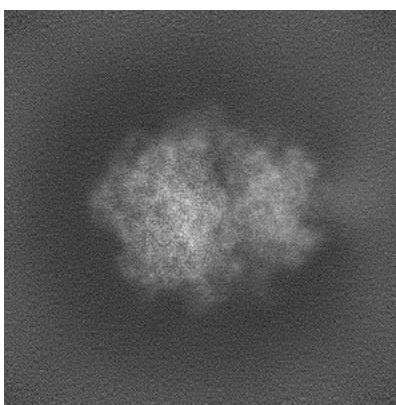


Z

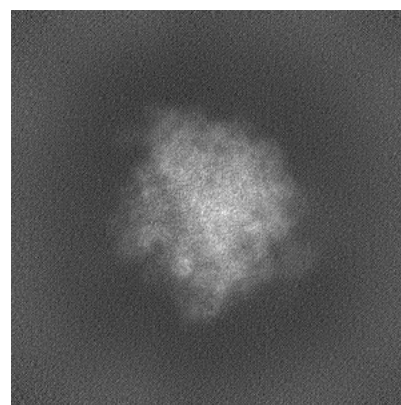
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 256

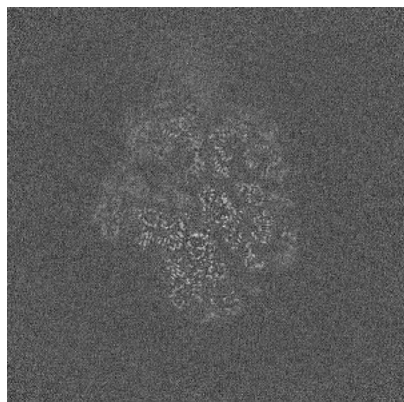


Y Index: 256

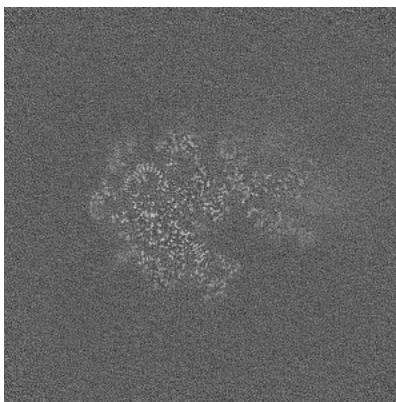


Z Index: 256

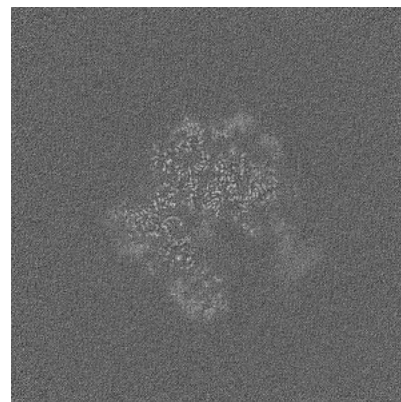
### 6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 270

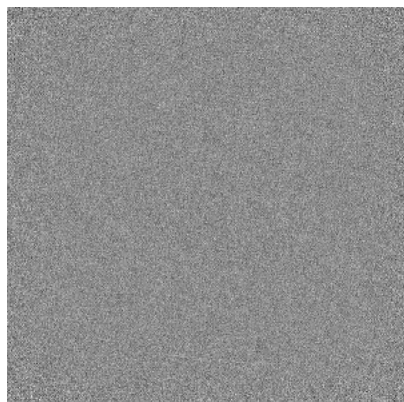


Y Index: 279

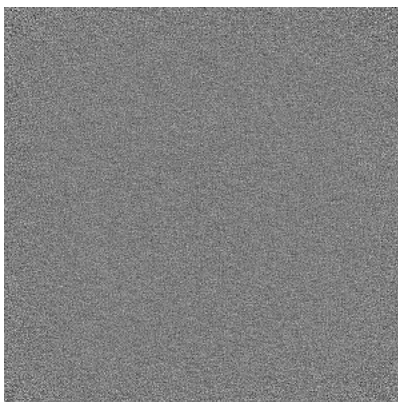


Z Index: 233

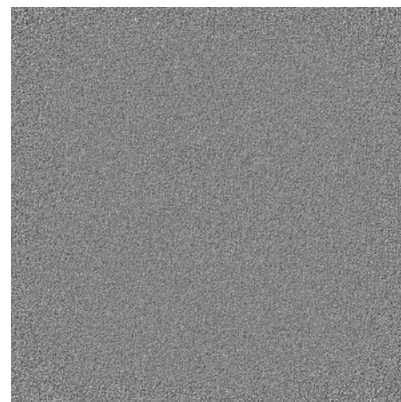
### 6.3.2 Raw map



X Index: 0



Y Index: 0



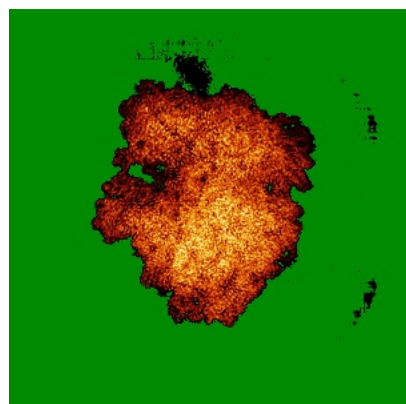
Z Index: 0

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

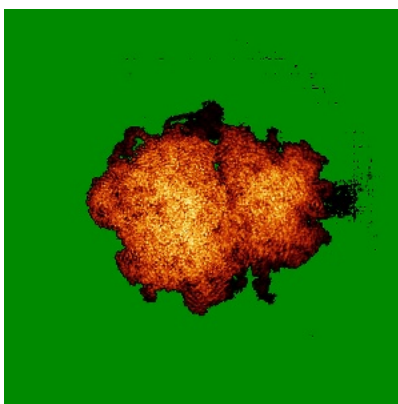


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

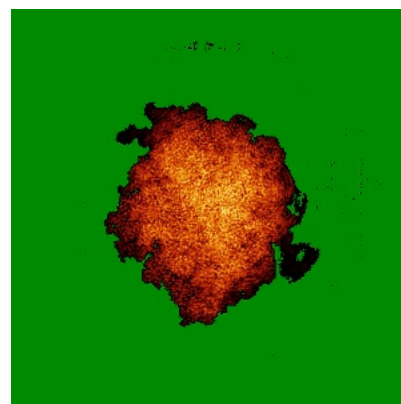
### 6.4.1 Primary map



X

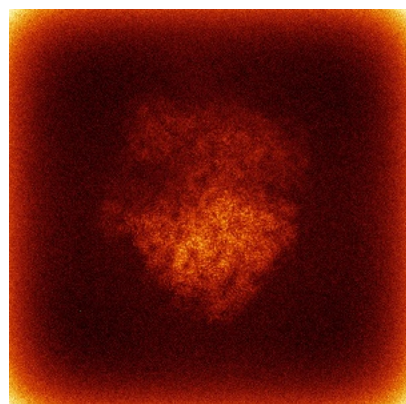


Y

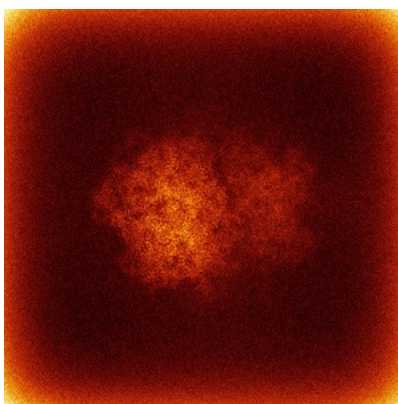


Z

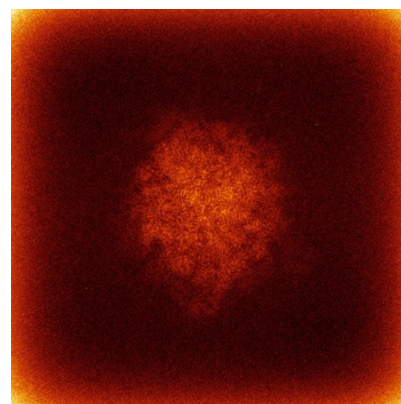
### 6.4.2 Raw map



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.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



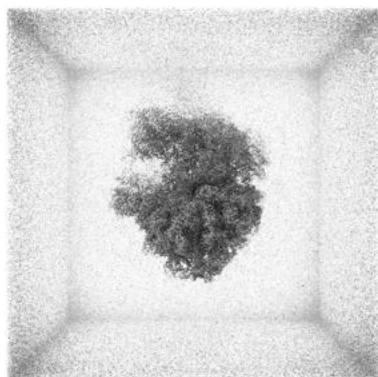
Y



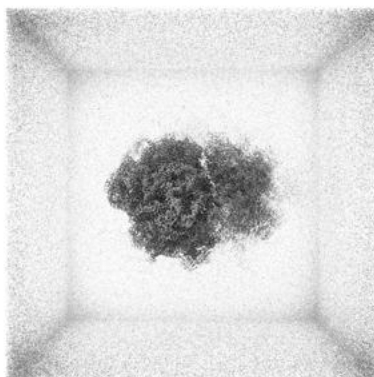
Z

The images above show the 3D surface view of the map at the recommended contour level 0.089. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

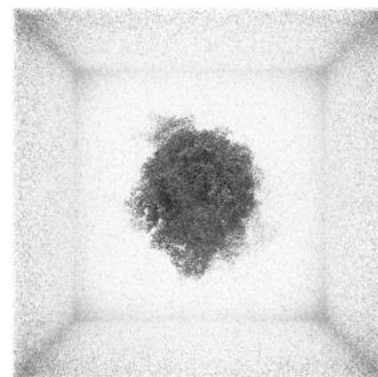
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

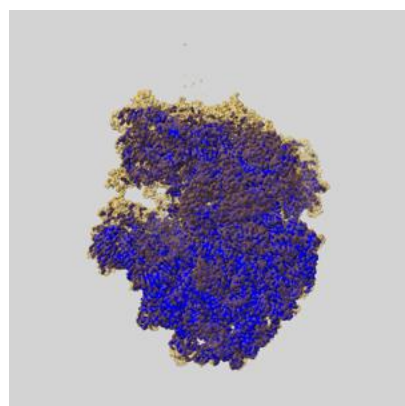
## 6.6 Mask visualisation [i](#)

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

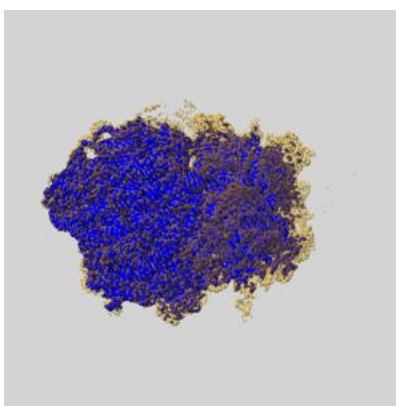
A mask typically either:

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

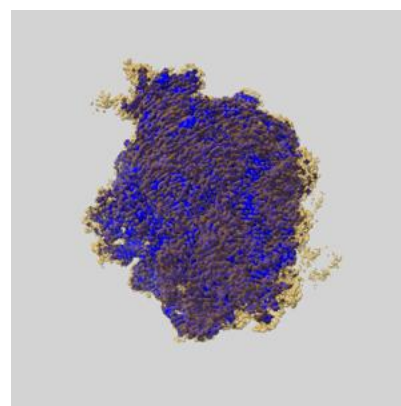
### 6.6.1 emd\_16047\_msk\_1.map [i](#)



X



Y

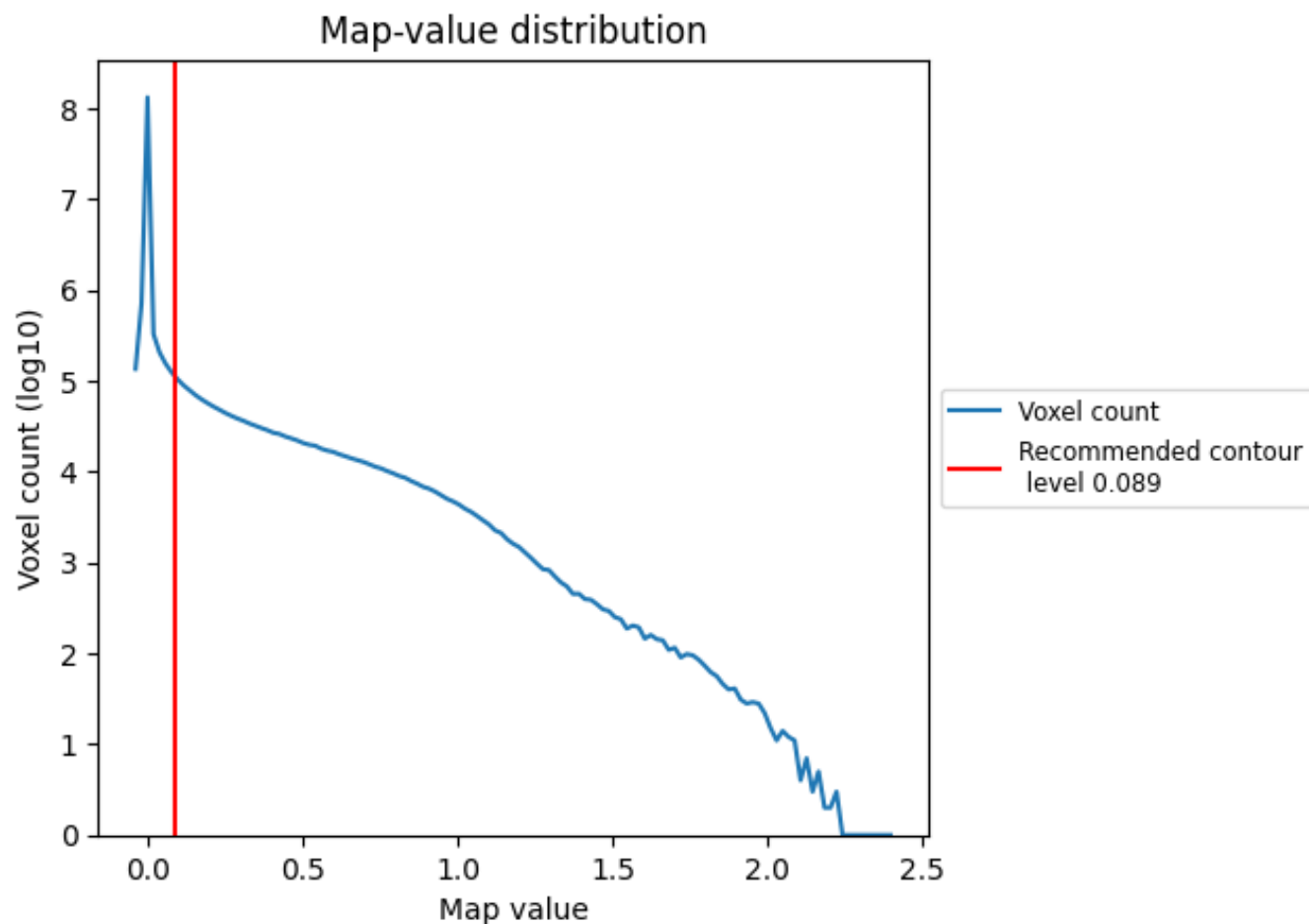


Z

## 7 Map analysis [i](#)

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

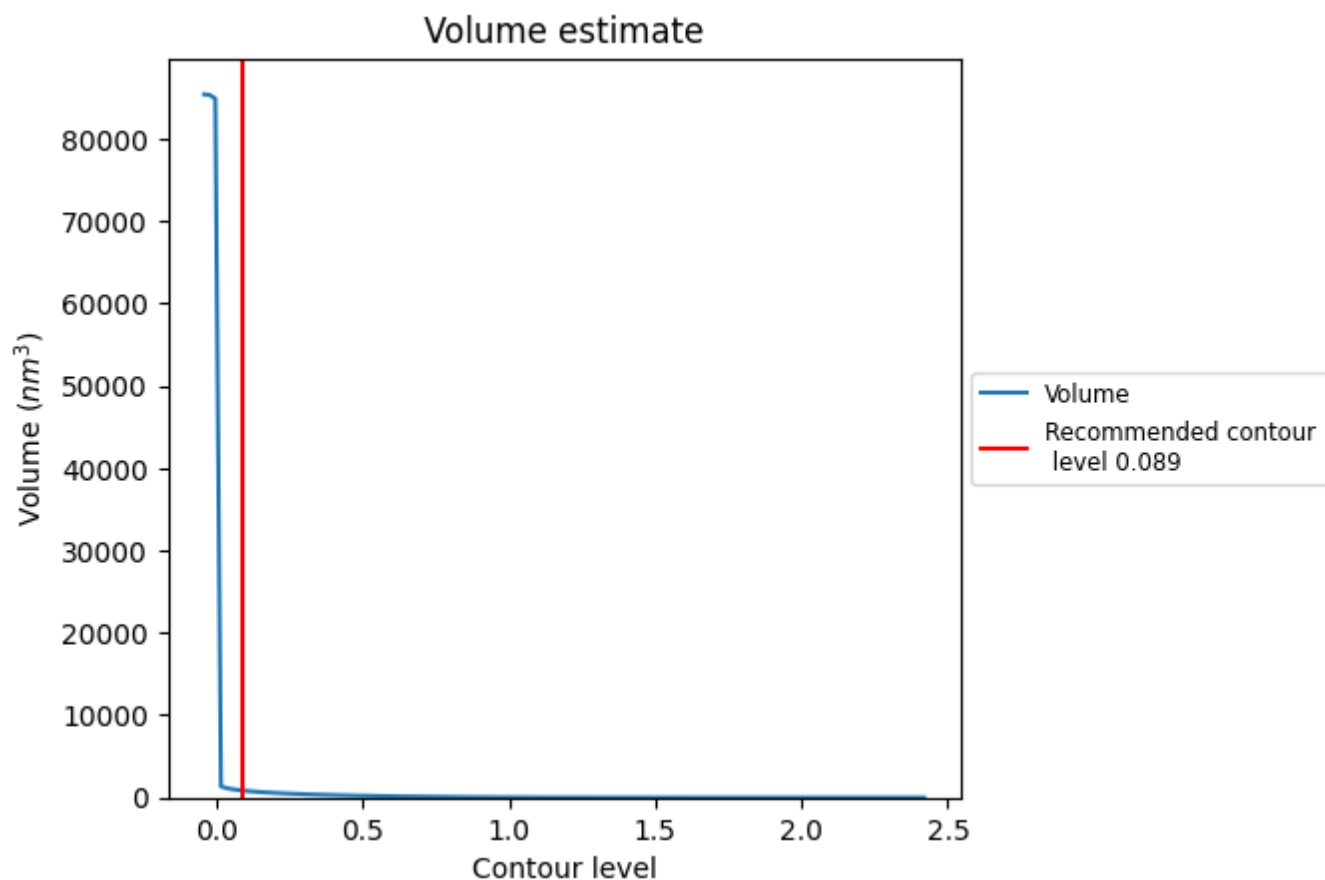
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



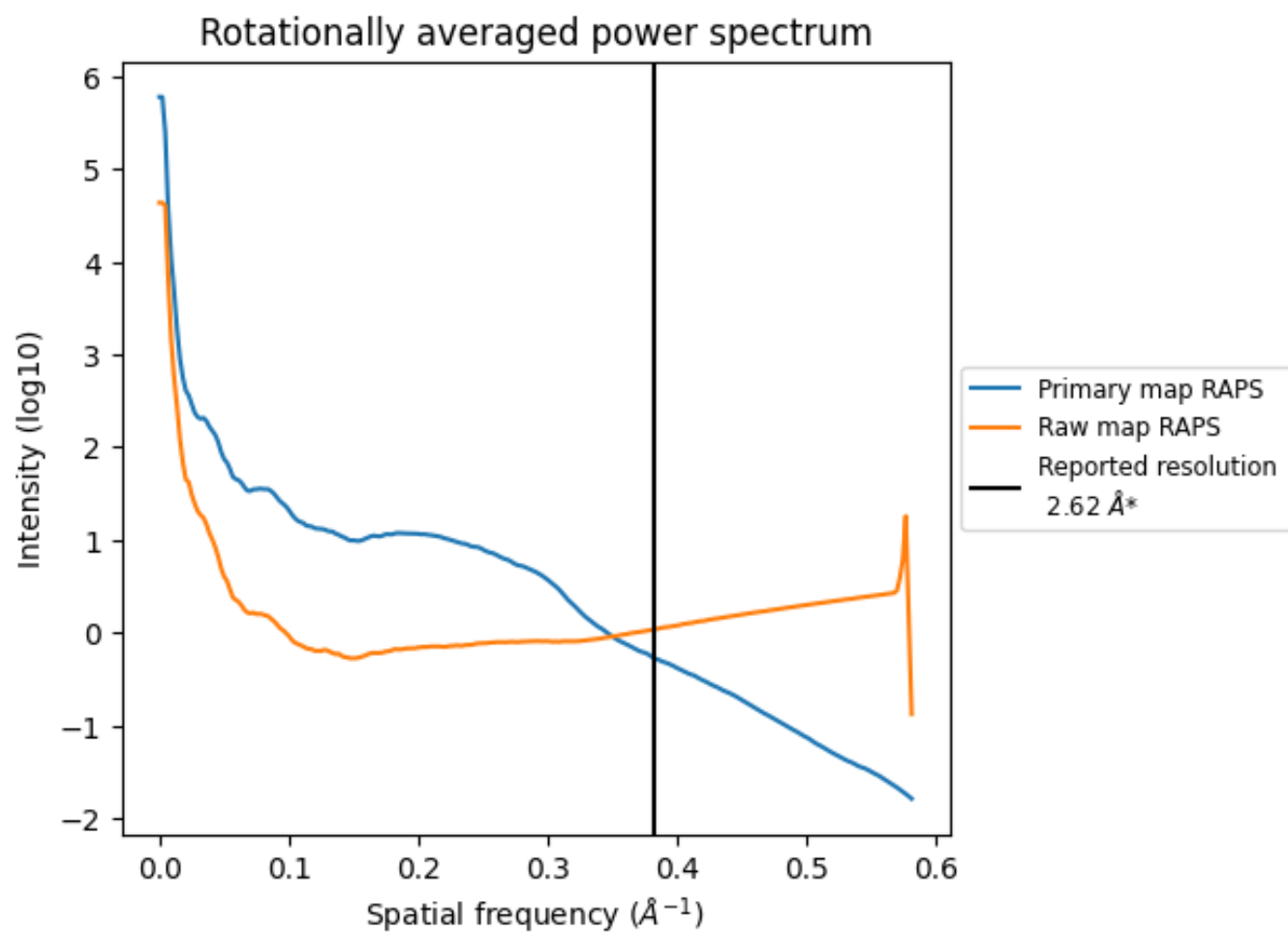
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 853 nm<sup>3</sup>; this corresponds to an approximate mass of 771 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 ⓘ

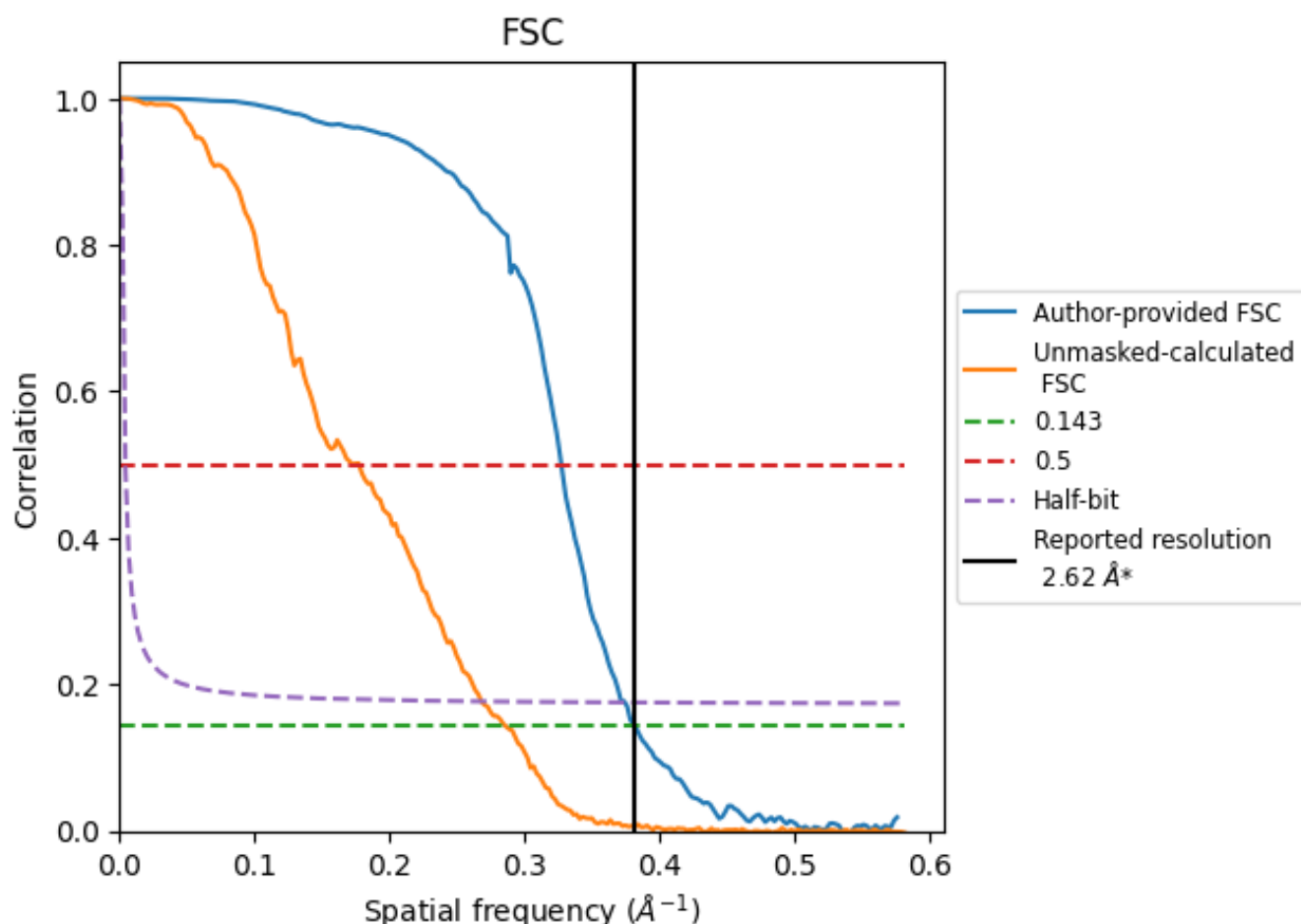


\*Reported resolution corresponds to spatial frequency of 0.382  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.382 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

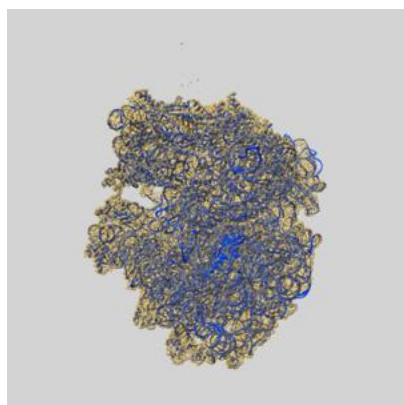
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.62	-	-
Author-provided FSC curve	2.62	3.06	2.67
Unmasked-calculated*	3.50	5.64	3.73

\*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 3.50 differs from the reported value 2.62 by more than 10 %

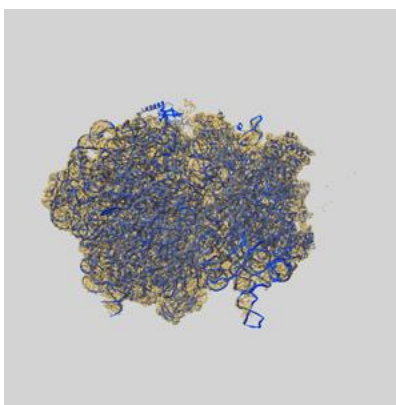
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16047 and PDB model 8BH4. Per-residue inclusion information can be found in section [3](#) on page [13](#).

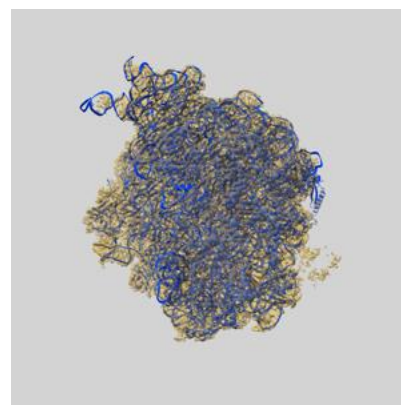
### 9.1 Map-model overlay [i](#)



X



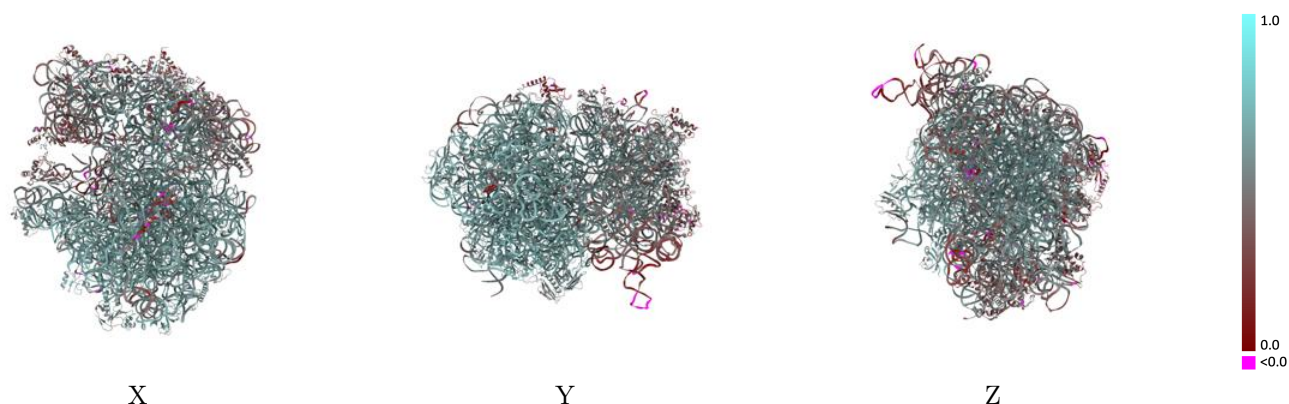
Y



Z

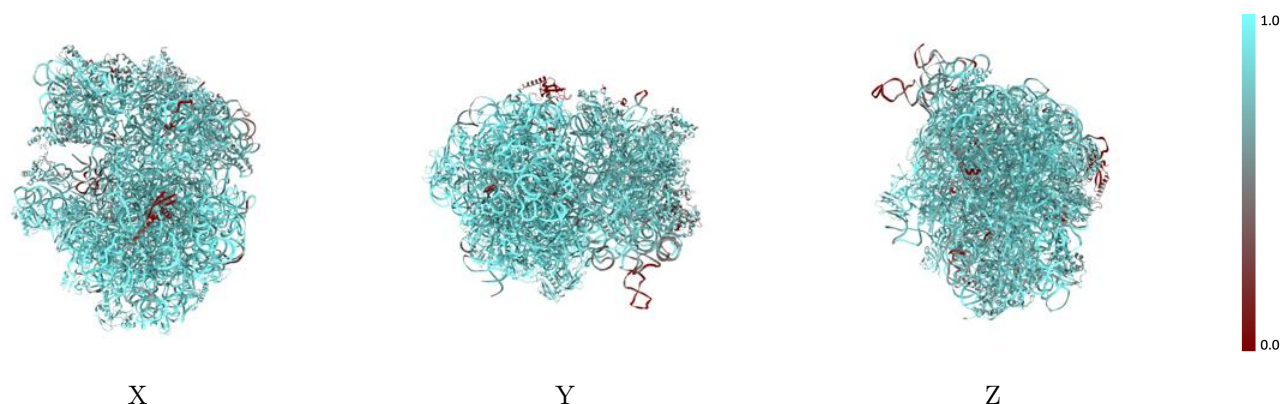
The images above show the 3D surface view of the map at the recommended contour level 0.089 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



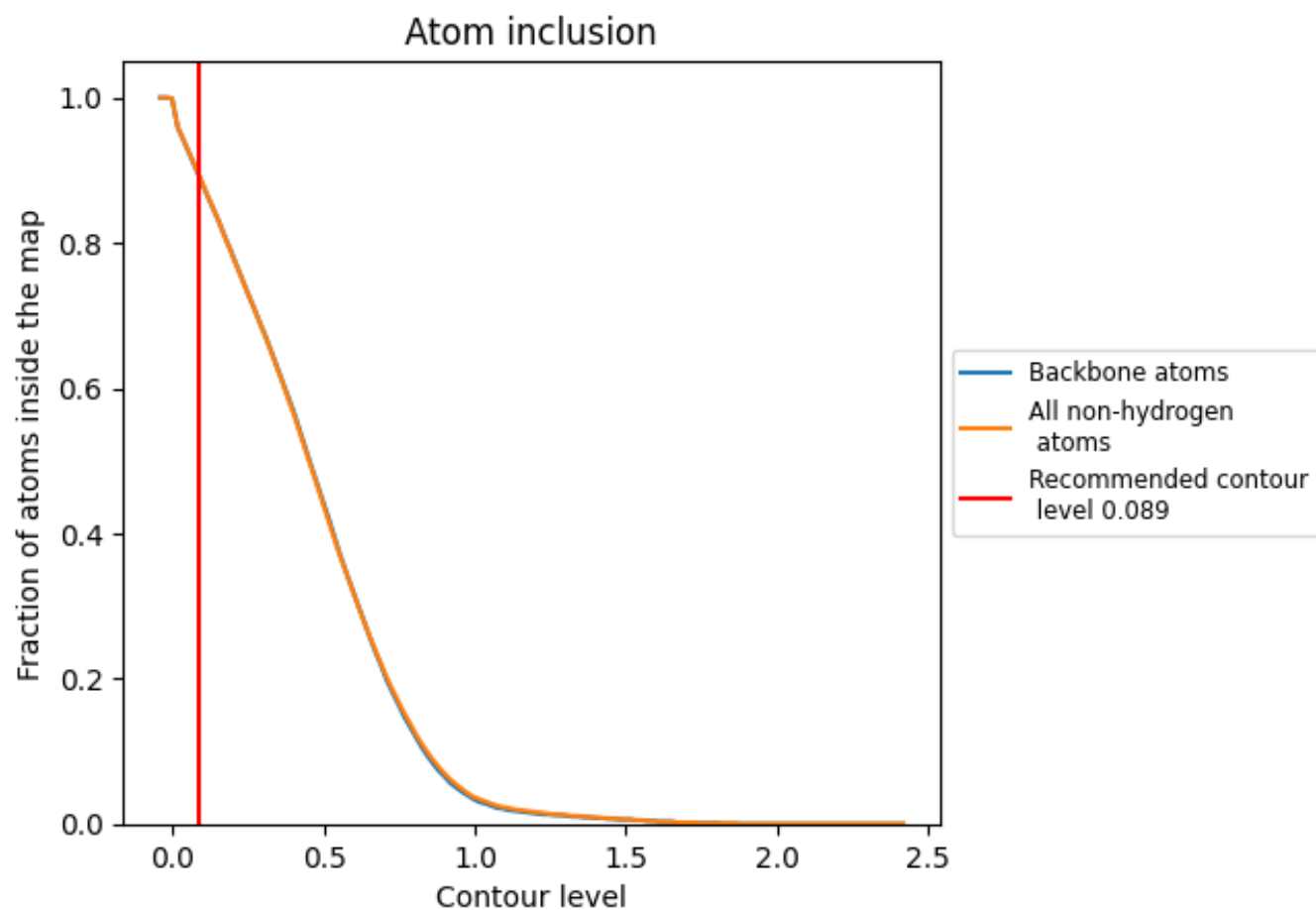
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 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 (0.089).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.089) and Q-score for the entire model and for each chain.











































Chain	Atom inclusion	Q-score
All	 0.8910	 0.5600
0	 0.9630	 0.6250
1	 0.9380	 0.5640
2	 0.8640	 0.4950
3	 0.9350	 0.6080
4	 0.6660	 0.4070
5	 0.8680	 0.5470
6	 0.6320	 0.5210
A	 0.9590	 0.6550
B	 0.9530	 0.6470
C	 0.9150	 0.6130
D	 0.6820	 0.3620
E	 0.8750	 0.5550
F	 0.2950	 0.2770
G	 0.9460	 0.6410
H	 0.9400	 0.6420
I	 0.9330	 0.6340
J	 0.9430	 0.6330
K	 0.9670	 0.6610
L	 0.8970	 0.5710
M	 0.9260	 0.6250
N	 0.9500	 0.6520
O	 0.9250	 0.6220
P	 0.9340	 0.6380
Q	 0.8960	 0.6060
R	 0.8890	 0.5980
S	 0.9000	 0.6020
T	 0.9390	 0.6460
U	 0.9330	 0.6320
V	 0.8850	 0.5730
W	 0.9370	 0.6320
a	 0.9350	 0.6490
b	 0.8700	 0.5860
c	 0.9550	 0.6630
d	 0.9550	 0.6570



*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
e	 0.9420	 0.6480
f	 0.7060	 0.4150
g	 0.8420	 0.5090
h	 0.5160	 0.3060
i	 0.8670	 0.5260
j	 0.7620	 0.4550
k	 0.6700	 0.3600
l	 0.8030	 0.4870
m	 0.7840	 0.4450
n	 0.7750	 0.4500
o	 0.8200	 0.5110
p	 0.8650	 0.5650
q	 0.7150	 0.3720
r	 0.8000	 0.4710
s	 0.7960	 0.4710
t	 0.7180	 0.4170
u	 0.7500	 0.4400
v	 0.6810	 0.4260
w	 0.6470	 0.3600
x	 0.8010	 0.4600
y	 0.6410	 0.3890