wwPDB EM Validation Summary Report (i)

Feb 25, 2024 – 12:14 AM EST

PDB ID	:	7JSW
EMDB ID	:	EMD-22461
Title	:	ArfB Rescue of a 70S Ribosome stalled on truncated mRNA with a partial A-site codon (+2-III)
Authors	:	Carbone, C.E.; Korostelev, A.A.
Deposited on	:	2020-08-16
Resolution	:	3.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

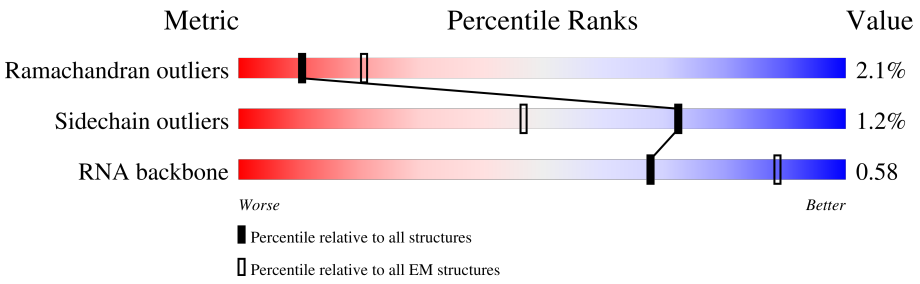
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	b	271	97% ·
2	c	209	99% ·
3	d	201	99% ·
4	e	177	· 97% ·
5	f	176	98% ·
6	g	149	93% 7%
7	j	142	98% ·
8	k	122	97% ·

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Mol	Chain	Length	Quality of chain
9	l	143	99%
10	m	136	99%
11	n	120	98%
12	o	116	99%
13	p	114	100%
14	q	117	98%
15	r	103	95% 5%
16	s	110	98%
17	t	93	99%
18	u	102	97%
19	v	94	97%
20	w	75	97%
21	x	77	100%
22	y	63	98%
23	z	58	98%
24	B	56	100%
25	C	50	98%
26	D	46	100%
27	E	64	98%
28	F	38	95% 5%
29	G	225	96%
30	H	206	98%
31	I	205	96%
32	J	157	96%
33	K	100	95% 5%

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Mol	Chain	Length	Quality of chain
34	L	151	98%
35	M	129	98%
36	N	127	94% 6%
37	O	98	93% 7%
38	P	116	98%
39	Q	123	97%
40	R	114	97%
41	S	100	93% 7%
42	T	88	95% 5%
43	U	82	96%
44	V	80	98%
45	W	65	98%
46	X	79	99%
47	Y	85	99%
48	Z	65	89% 11%
49	3	1539	86% 14%
50	1	2903	84% 16%
51	2	120	90% 10%
52	5	77	82% 18%
53	4	16	81% 19%
54	8	132	13% 81% 8% 9%

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 144808 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	b	271	2083	1288	423	365	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	c	209	1565	979	288	294	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	201	1552	974	283	290	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	e	177	1411	899	249	257	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	f	176	1323	832	243	246	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	g	149	1111	699	197	214	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	j	142	1129	714	212	199	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	k	122	939	587	180	166	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	l	143	1045	649	206	189	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	m	136	1074	686	205	177	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	n	120	961	593	196	167	5	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	o	116	892	552	178	162	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	p	114	917	574	179	163	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	q	117	947	604	192	151	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	r	103	816	516	153	145	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	s	110	857	532	166	156	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	t	93	739	466	139	132	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	u	102	780	492	146	142	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	v	94	753	479	137	134	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	w	75	575	356	116	102	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	x	77	625	388	129	106	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	y	63	509	313	99	95	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	z	58	449	281	87	79	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	B	56	444	269	94	80	1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	C	50	410	263	75	72	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	D	46	377	228	90	57	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	E	64	504	323	105	74	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	F	38	302	185	65	48	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	G	225	1757	1111	315	323	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	H	206	1625	1028	305	289	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	I	205	1643	1026	315	298	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	J	157	1157	719	218	214	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	K	100	818	515	148	149	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	L	151	1182	735	227	216	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	M	129	979	616	173	184	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	N	127	1022	634	206	179	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	O	98	787	493	150	143	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	P	116	870	535	173	159	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Q	123	955	590	196	165	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	R	114	884	546	178	157	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	S	100	805	499	164	139	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	T	88	714	439	144	130	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	U	82	649	406	128	114	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	V	80	649	411	121	114	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	W	65	536	339	100	96	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	X	79	638	408	120	108	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Y	85	665	411	137	114	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Z	65	545	335	117	92	1	0	0

- Molecule 49 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	3	1539	33012	14725	6053	10696	1538	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	1490	C	U	conflict	GB 1789840096

- Molecule 50 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	1	2903	62317	27801	11468	20146	2902	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

- Molecule 51 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	2	120	2568	1145	471	833	119	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 52 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
52	5	77	1640	732	297	535	76	0	0

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	4	16	353	158	74	105	16	0	0

- Molecule 54 is a protein called Peptidyl-tRNA hydrolase ArfB.

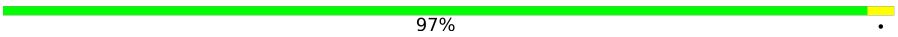
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	8	120	949	591	186	170	2	0	0

3 Residue-property plots (i)

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

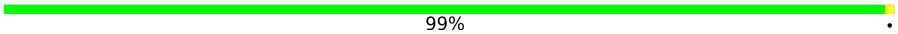
- Molecule 1: 50S ribosomal protein L2

Chain b:



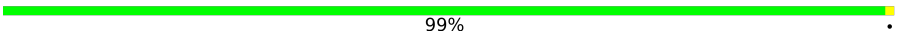
- Molecule 2: 50S ribosomal protein L3

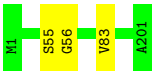
Chain c:



- Molecule 3: 50S ribosomal protein L4

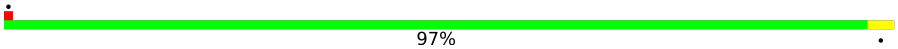
Chain d:

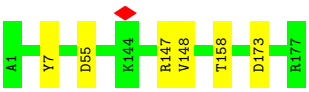




- Molecule 4: 50S ribosomal protein L5

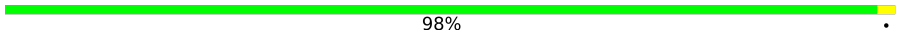
Chain e:

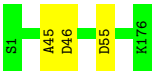




- Molecule 5: 50S ribosomal protein L6

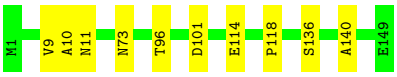
Chain f:





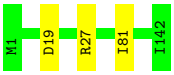
- Molecule 6: 50S ribosomal protein L9

Chain g: 93% 7%



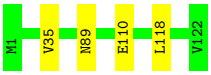
- Molecule 7: 50S ribosomal protein L13

Chain j: 98%



- Molecule 8: 50S ribosomal protein L14

Chain k: 97%



- Molecule 9: 50S ribosomal protein L15

Chain l: 99%

- Molecule 10: 50S ribosomal protein L16

Chain m: 99%

- Molecule 11: 50S ribosomal protein L17

Chain n: 98%

- Molecule 12: 50S ribosomal protein L18

Chain o: 99%

- Molecule 13: 50S ribosomal protein L19

Chain p: 100%

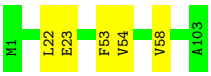
There are no outlier residues recorded for this chain.

• Molecule 14: 50S ribosomal protein L20

Chain q: 98%

• Molecule 15: 50S ribosomal protein L21

Chain r: 95% 5%



• Molecule 16: 50S ribosomal protein L22

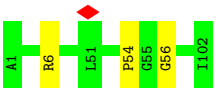
Chain s: 98%

• Molecule 17: 50S ribosomal protein L23

Chain t: 99%

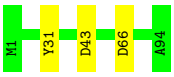
• Molecule 18: 50S ribosomal protein L24

Chain u: 97%



• Molecule 19: 50S ribosomal protein L25

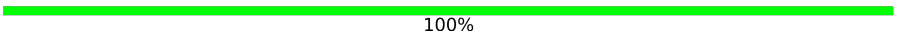
Chain v: 97%



• Molecule 20: 50S ribosomal protein L27

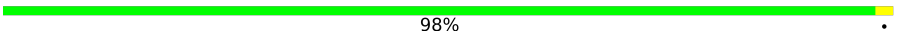
Chain w: 97%

• Molecule 21: 50S ribosomal protein L28

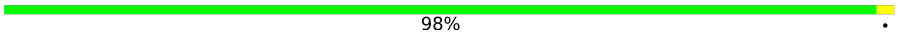
Chain x: 

There are no outlier residues recorded for this chain.

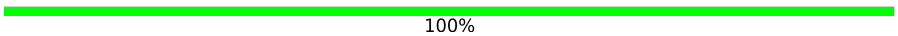
• Molecule 22: 50S ribosomal protein L29

Chain y: 

• Molecule 23: 50S ribosomal protein L30

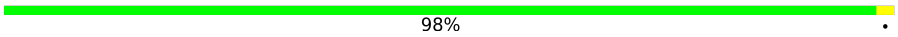
Chain z: 

• Molecule 24: 50S ribosomal protein L32

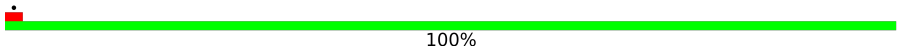
Chain B: 

There are no outlier residues recorded for this chain.

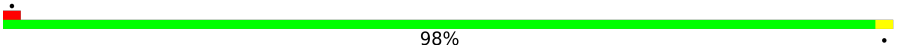
• Molecule 25: 50S ribosomal protein L33

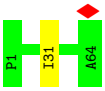
Chain C: 

• Molecule 26: 50S ribosomal protein L34

Chain D: 

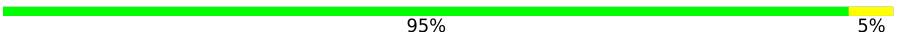
• Molecule 27: 50S ribosomal protein L35

Chain E: 



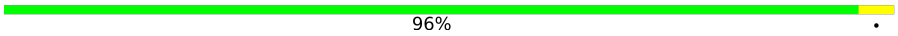
- Molecule 28: 50S ribosomal protein L36

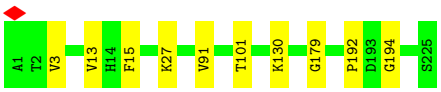
Chain F:



- Molecule 29: 30S ribosomal protein S2

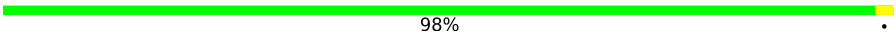
Chain G:





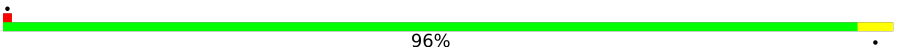
- Molecule 30: 30S ribosomal protein S3

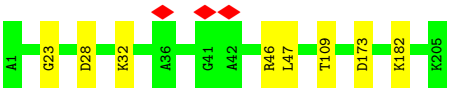
Chain H:



- Molecule 31: 30S ribosomal protein S4

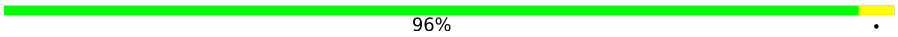
Chain I:





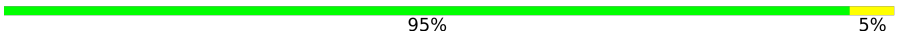
- Molecule 32: 30S ribosomal protein S5

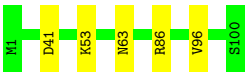
Chain J:



- Molecule 33: 30S ribosomal protein S6

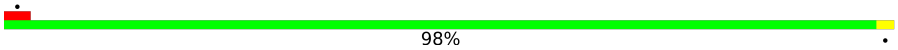
Chain K:

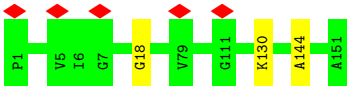




- Molecule 34: 30S ribosomal protein S7

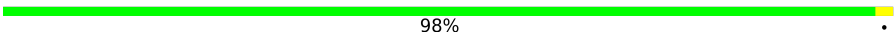
Chain L:

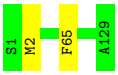




- Molecule 35: 30S ribosomal protein S8

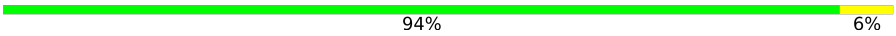
Chain M:

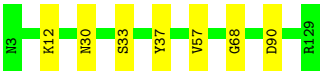




- Molecule 36: 30S ribosomal protein S9

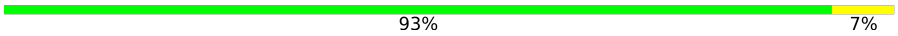
Chain N:

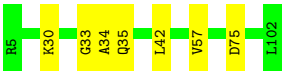




- Molecule 37: 30S ribosomal protein S10

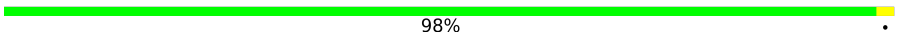
Chain O:





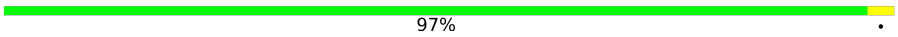
- Molecule 38: 30S ribosomal protein S11

Chain P:



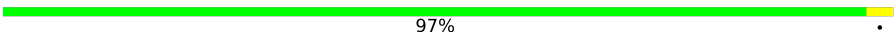
- Molecule 39: 30S ribosomal protein S12

Chain Q:



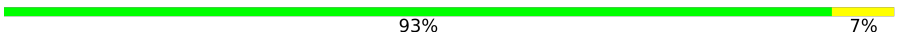
- Molecule 40: 30S ribosomal protein S13

Chain R:



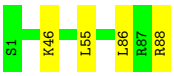
- Molecule 41: 30S ribosomal protein S14

Chain S:



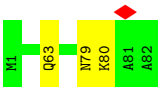
- Molecule 42: 30S ribosomal protein S15

Chain T: 95% 5%



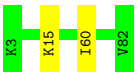
• Molecule 43: 30S ribosomal protein S16

Chain U: 96%



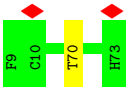
• Molecule 44: 30S ribosomal protein S17

Chain V: 98%



• Molecule 45: 30S ribosomal protein S18

Chain W: 98%



• Molecule 46: 30S ribosomal protein S19

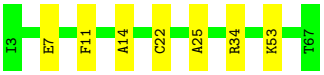
Chain X: 99%

• Molecule 47: 30S ribosomal protein S20

Chain Y: 99%

• Molecule 48: 30S ribosomal protein S21

Chain Z: 89% 11%



• Molecule 49: 16S ribosomal RNA

Chain 3: 86% 14%

A2 A3 U4 U5 G6 A7 A8 G9 G22 G31 A32 G39 C48 U49 A50 A51 G64 A65 A66 A71 G75 G76 G82 C83 U84 U92 U93 G94 G100 U121 A131 G141 G144 G145 G146 G168 U173 G177 C183 G184 A199

U208 U209 C210 G211 G212 U245 A246 G247 G251 G266 C267 G281 A282 U283 G289 C316 C328 U340 A344 C345 G346 G347 G348 C352 A356 U367 C372 U398 G406 G413 U421 C422 G423 G424 G428 U429 U438 G445 G446

G447 A448 A451 A452 G462 U467 A468 U479 U480 G481 G484 U485 U486 A496 G497 C518 G524 G527 A546 A547 U561 U562 A572 A573 A574 G575 C576 G577 A607 G615 G633 G654 G661 A665 A687 G688 U701 A702 G703

G713 A718 U723 G724 G733 G755 C758 A777 A794 A815 A816 C817 G818 A819 U820 G821 U842 U843 G844 A845 A846 G847 G902 A918 C934 A935 C940 U960 U961 G966 C967 A968 A969 C970 G971 A975 G976 A977 U992 G993 A1004

C1028 U1029 U1030 C1031 G1032 G1033 G1034 A1035 A1036 C1037 G1053 C1054 A1055 C1066 G1089 G1094 U1095 A1101 C1109 U1126 A1130 G1133 C1136 C1137 G1138 G1139 G1142 U1159 U1168 A1169 G1182 U1183 G1184 A1196 A1197 G1198 A1201 U1202 U1212 A1213 A1225 C1226

A1238 G1241 G1253 A1256 A1257 G1258 C1259 G1260 A1275 G1278 G1279 A1280 C1281 C1282 A1287 G1290 G1300 U1301 G1312 C1317 G1323 G1347 A1363 C1378 G1379 U1380 U1381 C1395 A1398 A1429 G1442 A1446 A1447 C1448 C1449 U1450 U1451 C1452 G1453 G1454

G1475 A1492 A1493 G1494 A1503 U1506 G1517 A1518 A1519 G1529 G1530 A1534 C1535 U1540

- Molecule 50: 23S ribosomal RNA

Chain 1: 84% 16%

G1 A10 C11 U12 U34 G35 G46 U50 G51 A63 A71 A74 G75 G80 A91 C96 U100 A101 G110 A118 A119 U120 U135 G136 U137 U138 U139 C140 G141 A142 U158 U162 C163 A181 A196 A199 A216 A219 G220

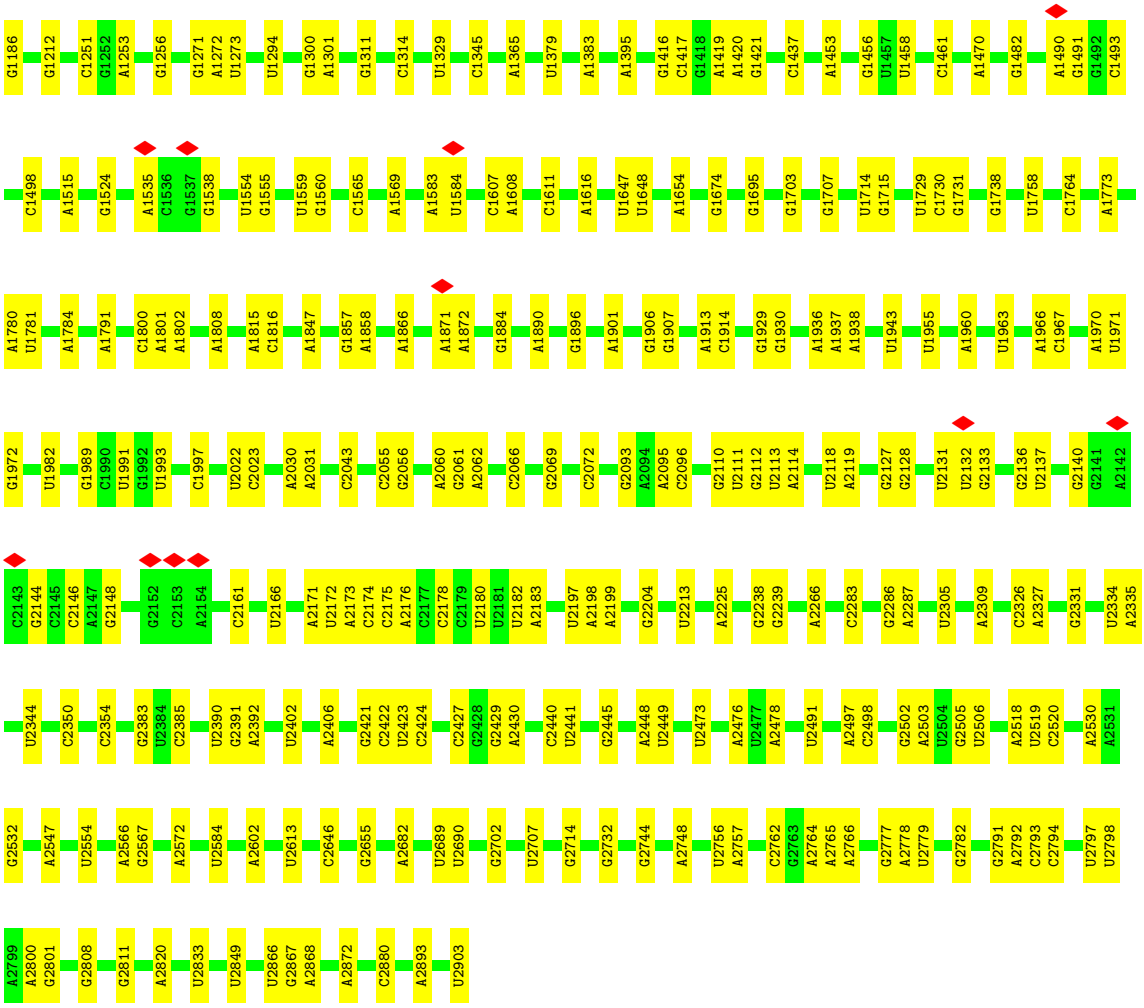
A221 A222 C228 A233 A241 G248 C249 G250 A255 G266 U276 G277 A278 A279 U280 C281 A282 G285 U286 G287 A294 C302 A310 A311 G312 G317 C318 G319 C323 A324 G329 A330 A362 G367 A371 G372 U387 G388 G389 U390 A391

A404 U405 G406 G411 A412 C421 A422 A423 G424 U437 C455 A480 G481 C490 G491 A504 A505 A508 G529 A532 G533 C544 U545 U546 A547 G548 G549 C550 A563 U573 A574 A575 A603 A627 G628 A637 U646 G651 A654 G669

A675 U686 G687 G695 G704 A705 G711 A730 C747 G748 A749 A752 A764 C765 G774 G775 G776 G777 A782 A783 G784 G785 A800 G805 C812 A819 A825 U826 U827 U828 A829 G830 A844 A845 U846 U847 G856 G859 U860 A866

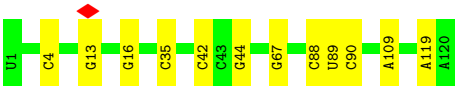
A878 U887 C888 C889 A896 C897 A900 G907 A910 C915 U932 A933 A941 C946 C961 A973 G974 A983 C995 A996 U1012 C1013 A1020 A1021 G1022 G1026 U1033 A1046 A1057 U1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068

A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 U1082 U1083 A1084 G1087 A1088 A1089 A1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 A1111 U1130 G1131 U1132 A1133 A1134 C1135 G1136 U1141 A1142 A1143 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181



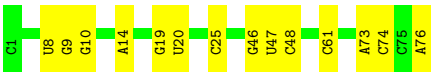
- Molecule 51: 5S ribosomal RNA

Chain 2:



- Molecule 52: tRNAfMet

Chain 5:

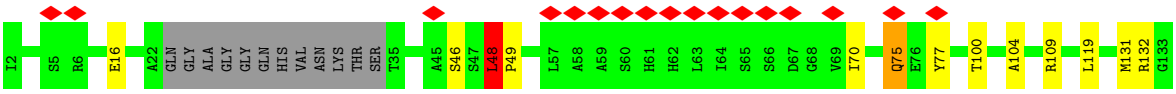


- Molecule 53: mRNA

Chain 4:

• Molecule 54: Peptidyl-tRNA hydrolase ArfB

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7464	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	30.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	12.365	Depositor
Minimum map value	-5.856	Depositor
Average map value	0.096	Depositor
Map value standard deviation	0.614	Depositor
Recommended contour level	0.592	Depositor
Map size (Å)	389.76, 389.76, 389.76	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	b	0.25	0/2122	0.54	0/2852
2	c	0.28	0/1586	0.53	0/2134
3	d	0.27	0/1571	0.51	0/2113
4	e	0.31	0/1435	0.56	0/1926
5	f	0.27	0/1343	0.54	0/1816
6	g	0.29	0/1122	0.57	0/1515
7	j	0.27	0/1152	0.53	0/1551
8	k	0.27	0/948	0.58	0/1268
9	l	0.27	0/1054	0.57	0/1403
10	m	0.29	0/1093	0.54	0/1460
11	n	0.28	0/974	0.51	0/1301
12	o	0.27	0/902	0.52	0/1209
13	p	0.27	0/929	0.51	0/1242
14	q	0.29	0/960	0.47	0/1278
15	r	0.30	0/829	0.58	0/1107
16	s	0.25	0/864	0.55	0/1156
17	t	0.26	0/745	0.53	0/994
18	u	0.29	0/788	0.53	0/1051
19	v	0.28	0/766	0.53	0/1025
20	w	0.30	0/582	0.51	0/769
21	x	0.28	0/635	0.55	0/848
22	y	0.27	0/510	0.50	0/677
23	z	0.26	0/453	0.56	0/605
24	B	0.25	0/450	0.50	0/599
25	C	0.30	0/417	0.52	0/554
26	D	0.29	0/380	0.55	0/498
27	E	0.29	0/513	0.54	0/676
28	F	0.26	0/303	0.49	0/397
29	G	0.30	0/1788	0.56	1/2408 (0.0%)
30	H	0.28	0/1652	0.53	0/2225
31	I	0.28	0/1665	0.54	0/2227
32	J	0.28	0/1170	0.57	0/1573
33	K	0.29	0/836	0.57	0/1128
34	L	0.28	0/1196	0.51	0/1602

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	M	0.27	0/989	0.54	0/1326
36	N	0.29	0/1034	0.59	0/1375
37	O	0.27	0/797	0.57	0/1077
38	P	0.29	0/886	0.52	0/1195
39	Q	0.27	0/969	0.61	0/1300
40	R	0.27	0/893	0.59	0/1193
41	S	0.28	0/817	0.56	0/1088
42	T	0.27	0/722	0.56	0/964
43	U	0.30	0/659	0.53	0/884
44	V	0.28	0/658	0.57	0/881
45	W	0.31	0/545	0.56	0/731
46	X	0.31	0/653	0.52	0/877
47	Y	0.27	0/671	0.49	0/888
48	Z	0.32	0/551	0.64	0/728
49	3	0.28	0/36963	0.64	0/57662
50	1	0.28	0/69796	0.64	0/108888
51	2	0.29	0/2872	0.65	0/4479
52	5	0.29	0/1832	0.65	0/2855
53	4	0.37	0/398	0.65	0/620
54	8	0.30	0/959	0.69	1/1285 (0.1%)
All	All	0.28	0/157397	0.62	2/235483 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	G	194	GLY	N-CA-C	-5.37	99.67	113.10
54	8	48	LEU	N-CA-C	-5.30	96.68	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	269/271 (99%)	227 (84%)	38 (14%)	4 (2%)	10	46
2	c	207/209 (99%)	183 (88%)	22 (11%)	2 (1%)	15	52
3	d	199/201 (99%)	166 (83%)	30 (15%)	3 (2%)	10	46
4	e	175/177 (99%)	139 (79%)	31 (18%)	5 (3%)	4	34
5	f	174/176 (99%)	151 (87%)	21 (12%)	2 (1%)	14	51
6	g	147/149 (99%)	118 (80%)	21 (14%)	8 (5%)	2	22
7	j	140/142 (99%)	130 (93%)	9 (6%)	1 (1%)	22	60
8	k	120/122 (98%)	102 (85%)	15 (12%)	3 (2%)	5	36
9	l	141/143 (99%)	114 (81%)	26 (18%)	1 (1%)	22	60
10	m	134/136 (98%)	117 (87%)	16 (12%)	1 (1%)	22	60
11	n	118/120 (98%)	103 (87%)	15 (13%)	0	100	100
12	o	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	17	54
13	p	112/114 (98%)	91 (81%)	21 (19%)	0	100	100
14	q	115/117 (98%)	106 (92%)	8 (7%)	1 (1%)	17	54
15	r	101/103 (98%)	72 (71%)	26 (26%)	3 (3%)	4	33
16	s	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	8	42
17	t	91/93 (98%)	75 (82%)	15 (16%)	1 (1%)	14	51
18	u	100/102 (98%)	78 (78%)	19 (19%)	3 (3%)	4	33
19	v	92/94 (98%)	80 (87%)	10 (11%)	2 (2%)	6	39
20	w	73/75 (97%)	63 (86%)	9 (12%)	1 (1%)	11	46
21	x	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
22	y	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	9	44
23	z	56/58 (97%)	47 (84%)	9 (16%)	0	100	100
24	B	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
25	C	48/50 (96%)	37 (77%)	11 (23%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	D	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
27	E	62/64 (97%)	53 (86%)	8 (13%)	1 (2%)	9	44
28	F	36/38 (95%)	29 (81%)	6 (17%)	1 (3%)	5	35
29	G	223/225 (99%)	186 (83%)	30 (14%)	7 (3%)	4	33
30	H	204/206 (99%)	175 (86%)	25 (12%)	4 (2%)	7	41
31	I	203/205 (99%)	169 (83%)	29 (14%)	5 (2%)	5	36
32	J	155/157 (99%)	124 (80%)	27 (17%)	4 (3%)	5	36
33	K	98/100 (98%)	68 (69%)	26 (26%)	4 (4%)	3	27
34	L	149/151 (99%)	130 (87%)	17 (11%)	2 (1%)	12	48
35	M	127/129 (98%)	112 (88%)	14 (11%)	1 (1%)	19	57
36	N	125/127 (98%)	94 (75%)	25 (20%)	6 (5%)	2	24
37	O	96/98 (98%)	77 (80%)	13 (14%)	6 (6%)	1	20
38	P	114/116 (98%)	94 (82%)	18 (16%)	2 (2%)	8	42
39	Q	121/123 (98%)	90 (74%)	28 (23%)	3 (2%)	5	36
40	R	112/114 (98%)	97 (87%)	13 (12%)	2 (2%)	8	42
41	S	98/100 (98%)	77 (79%)	15 (15%)	6 (6%)	1	20
42	T	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	13	50
43	U	80/82 (98%)	68 (85%)	10 (12%)	2 (2%)	5	36
44	V	78/80 (98%)	68 (87%)	9 (12%)	1 (1%)	12	48
45	W	63/65 (97%)	56 (89%)	6 (10%)	1 (2%)	9	44
46	X	77/79 (98%)	66 (86%)	11 (14%)	0	100	100
47	Y	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
48	Z	63/65 (97%)	47 (75%)	12 (19%)	4 (6%)	1	20
54	8	116/132 (88%)	84 (72%)	23 (20%)	9 (8%)	1	15
All	All	5637/5749 (98%)	4732 (84%)	788 (14%)	117 (2%)	10	40

5 of 117 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	83	VAL
7	j	81	ILE
8	k	89	ASN
8	k	110	GLU
12	o	34	HIS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	216/216 (100%)	212 (98%)	4 (2%)	57	76
2	c	164/164 (100%)	163 (99%)	1 (1%)	86	92
3	d	165/165 (100%)	165 (100%)	0	100	100
4	e	148/148 (100%)	147 (99%)	1 (1%)	84	91
5	f	137/137 (100%)	136 (99%)	1 (1%)	84	91
6	g	114/114 (100%)	112 (98%)	2 (2%)	59	77
7	j	116/116 (100%)	114 (98%)	2 (2%)	60	78
8	k	103/103 (100%)	102 (99%)	1 (1%)	76	86
9	l	102/102 (100%)	102 (100%)	0	100	100
10	m	109/109 (100%)	109 (100%)	0	100	100
11	n	100/100 (100%)	98 (98%)	2 (2%)	55	75
12	o	86/86 (100%)	85 (99%)	1 (1%)	71	84
13	p	99/99 (100%)	99 (100%)	0	100	100
14	q	89/89 (100%)	88 (99%)	1 (1%)	73	85
15	r	84/84 (100%)	82 (98%)	2 (2%)	49	71
16	s	93/93 (100%)	93 (100%)	0	100	100
17	t	80/80 (100%)	80 (100%)	0	100	100
18	u	83/83 (100%)	83 (100%)	0	100	100
19	v	78/78 (100%)	77 (99%)	1 (1%)	69	82
20	w	57/57 (100%)	56 (98%)	1 (2%)	59	77
21	x	67/67 (100%)	67 (100%)	0	100	100
22	y	55/55 (100%)	55 (100%)	0	100	100
23	z	48/48 (100%)	47 (98%)	1 (2%)	53	74
24	B	47/47 (100%)	47 (100%)	0	100	100
25	C	45/45 (100%)	44 (98%)	1 (2%)	52	72
26	D	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	E	51/51 (100%)	51 (100%)	0	100	100
28	F	34/34 (100%)	33 (97%)	1 (3%)	42	67
29	G	186/186 (100%)	184 (99%)	2 (1%)	73	85
30	H	170/170 (100%)	169 (99%)	1 (1%)	86	92
31	I	172/172 (100%)	169 (98%)	3 (2%)	60	78
32	J	119/119 (100%)	117 (98%)	2 (2%)	60	78
33	K	87/87 (100%)	86 (99%)	1 (1%)	73	85
34	L	124/124 (100%)	123 (99%)	1 (1%)	81	89
35	M	104/104 (100%)	103 (99%)	1 (1%)	76	86
36	N	105/105 (100%)	104 (99%)	1 (1%)	76	86
37	O	86/86 (100%)	85 (99%)	1 (1%)	71	84
38	P	89/89 (100%)	89 (100%)	0	100	100
39	Q	103/103 (100%)	102 (99%)	1 (1%)	76	86
40	R	92/92 (100%)	91 (99%)	1 (1%)	73	85
41	S	83/83 (100%)	82 (99%)	1 (1%)	71	84
42	T	76/76 (100%)	73 (96%)	3 (4%)	32	60
43	U	65/65 (100%)	64 (98%)	1 (2%)	65	81
44	V	74/74 (100%)	73 (99%)	1 (1%)	67	81
45	W	56/56 (100%)	56 (100%)	0	100	100
46	X	70/70 (100%)	69 (99%)	1 (1%)	67	81
47	Y	65/65 (100%)	64 (98%)	1 (2%)	65	81
48	Z	55/55 (100%)	52 (94%)	3 (6%)	21	53
54	8	100/108 (93%)	94 (94%)	6 (6%)	19	50
All	All	4689/4697 (100%)	4634 (99%)	55 (1%)	72	84

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	I	173	ASP
37	O	30	LYS
54	8	119	LEU
54	8	16	GLU
32	J	55	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
17	t	92	ASN
29	G	202	ASN
54	8	62	HIS
45	W	30	ASN
18	u	73	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	3	1538/1539 (99%)	222 (14%)	0
50	1	2902/2903 (99%)	454 (15%)	10 (0%)
51	2	119/120 (99%)	12 (10%)	0
52	5	76/77 (98%)	14 (18%)	0
53	4	15/16 (93%)	3 (20%)	0
All	All	4650/4655 (99%)	705 (15%)	10 (0%)

5 of 705 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
49	3	4	U
49	3	6	G
49	3	8	A
49	3	9	G
49	3	22	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
50	1	2326	C
50	1	2391	G
50	1	2756	U
50	1	1020	A
50	1	1130	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

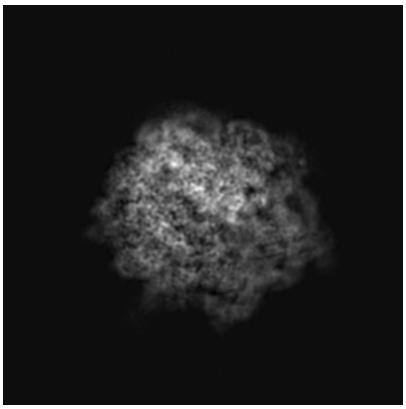
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22461. These allow visual inspection of the internal detail of the map and identification of artifacts.

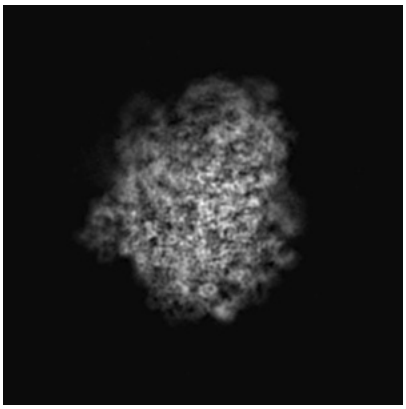
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

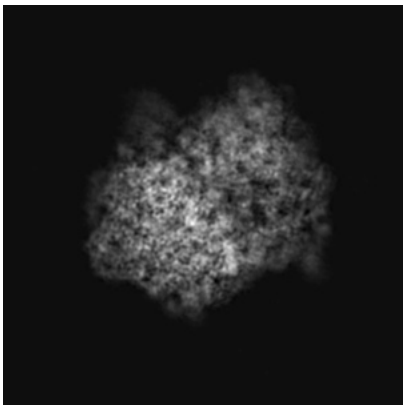
6.1.1 Primary map



X

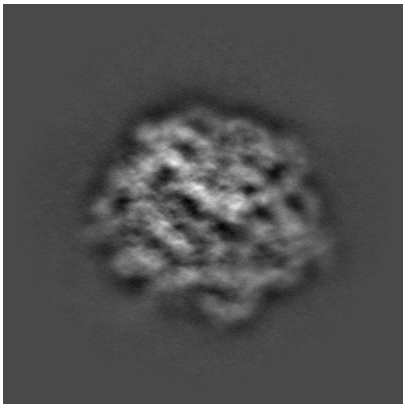


Y

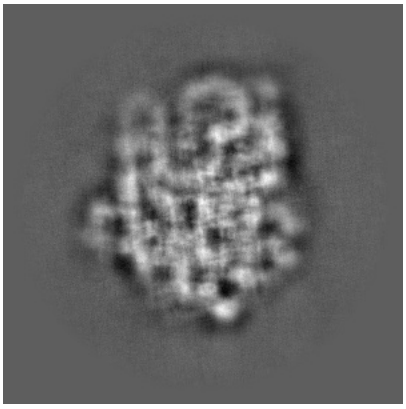


Z

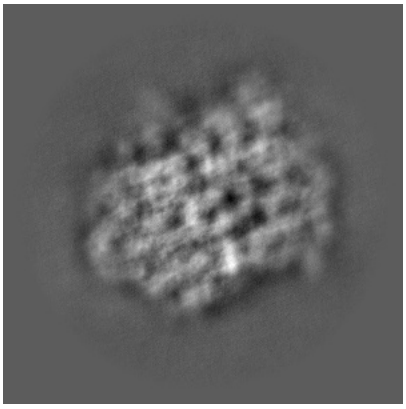
6.1.2 Raw map



X



Y

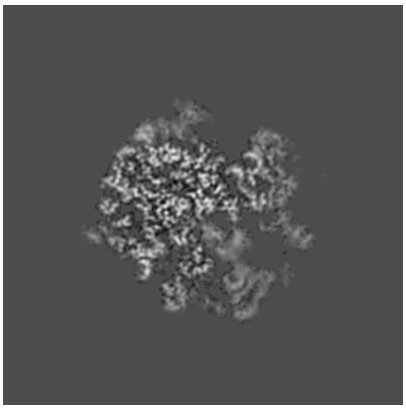


Z

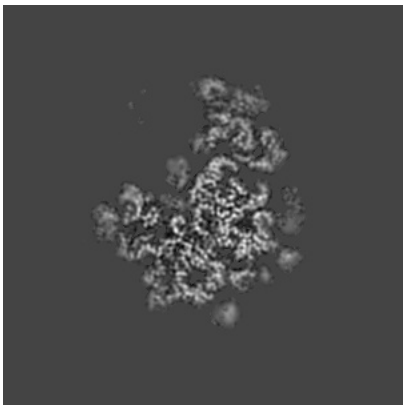
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

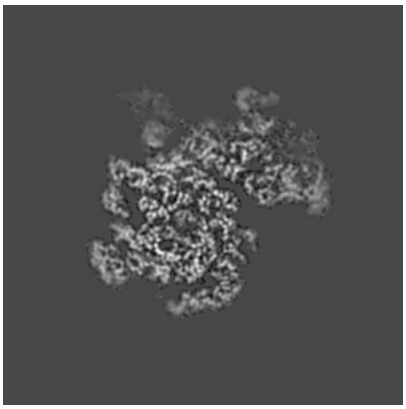
6.2.1 Primary map



X Index: 224

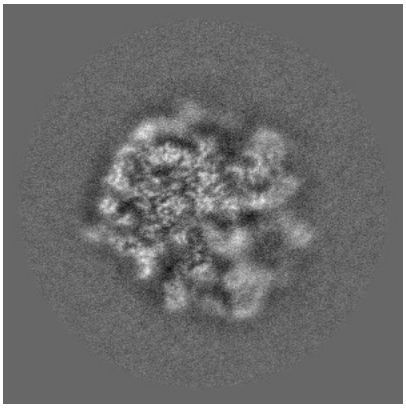


Y Index: 224

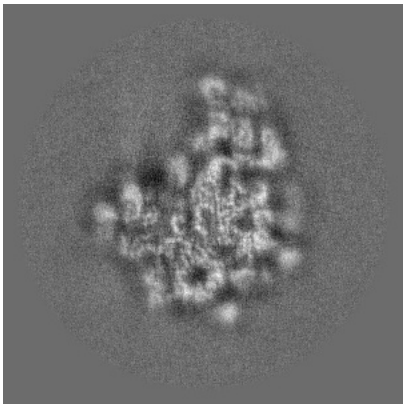


Z Index: 224

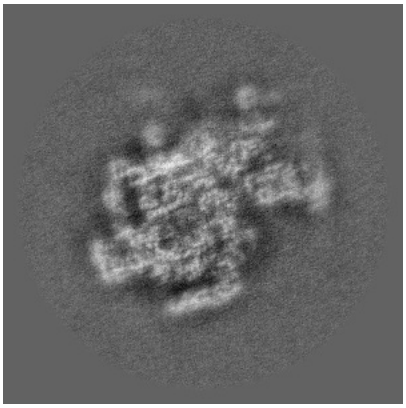
6.2.2 Raw map



X Index: 224



Y Index: 224

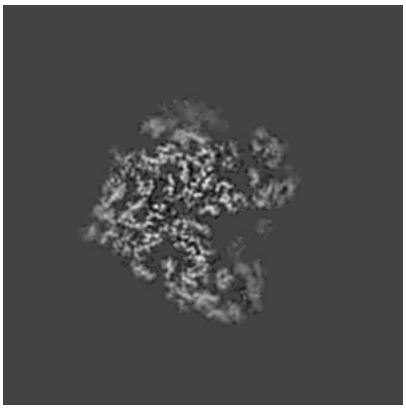


Z Index: 224

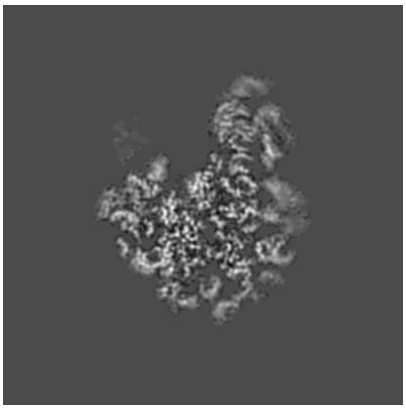
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

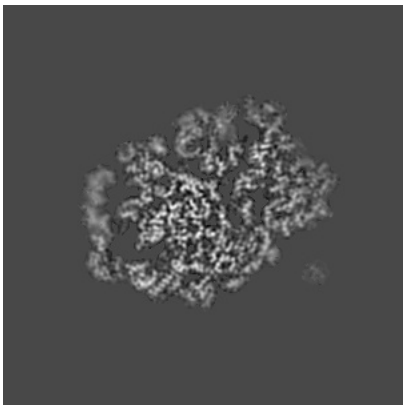
6.3.1 Primary map



X Index: 211

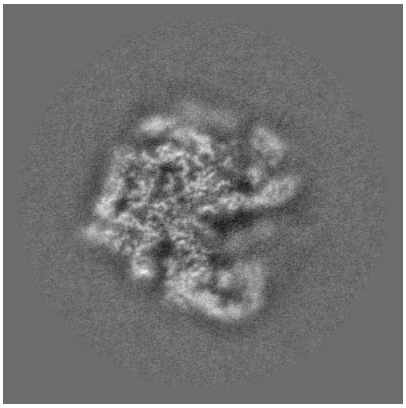


Y Index: 201

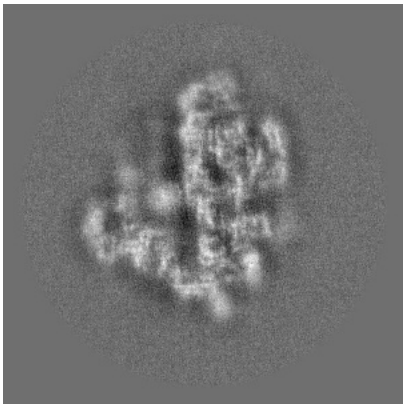


Z Index: 246

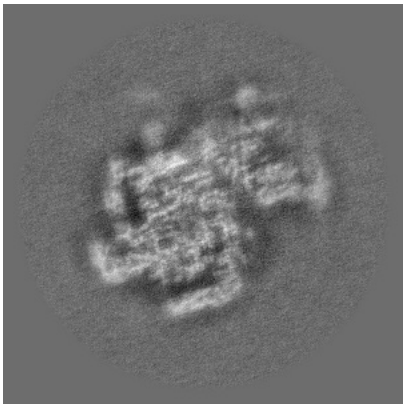
6.3.2 Raw map



X Index: 213



Y Index: 257

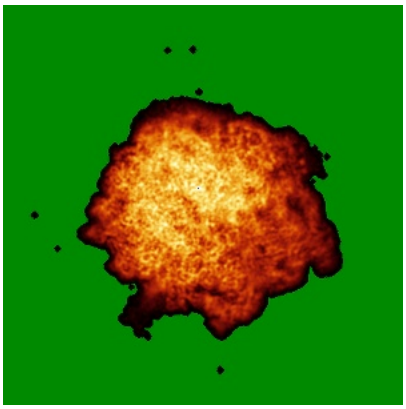


Z Index: 222

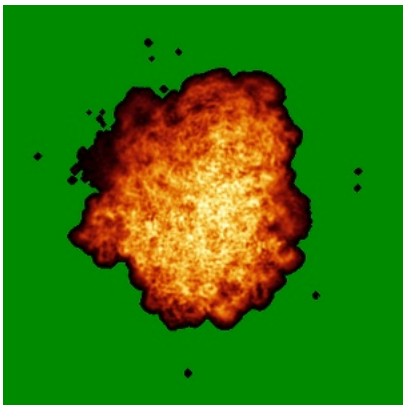
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

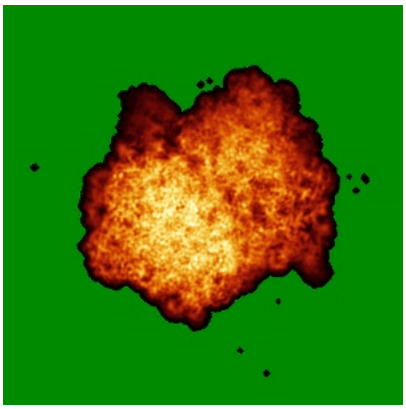
6.4.1 Primary map



X

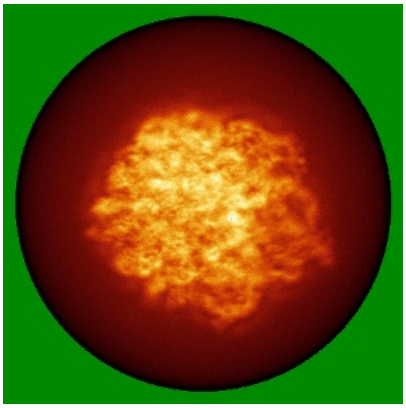


Y

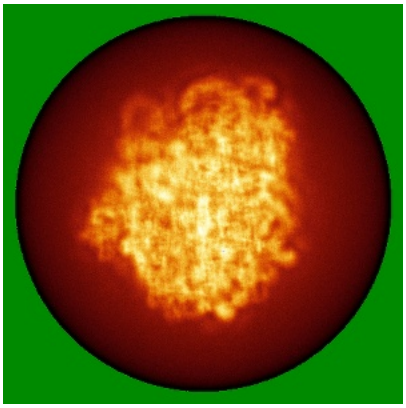


Z

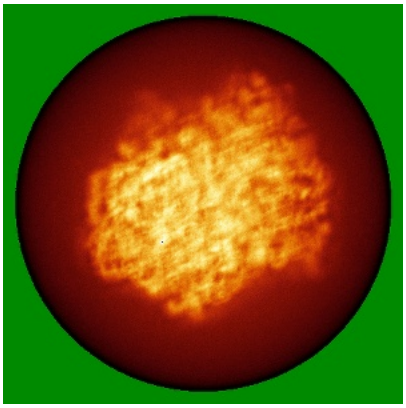
6.4.2 Raw map



X



Y

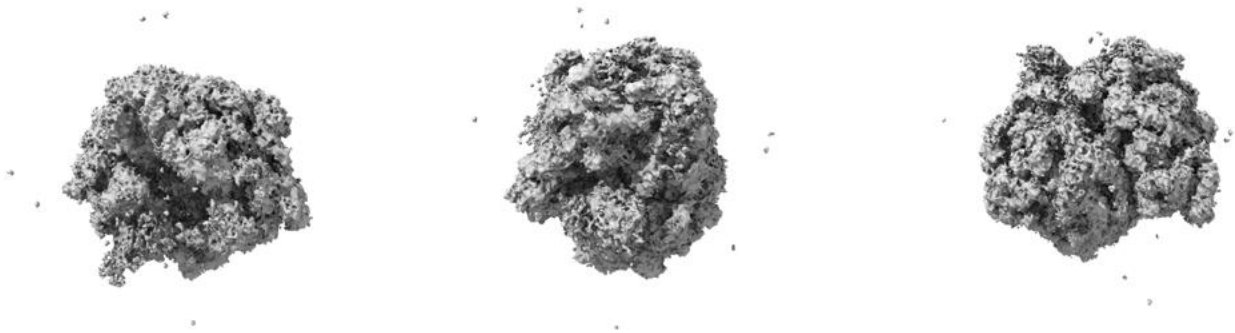


Z

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 0.592. 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.

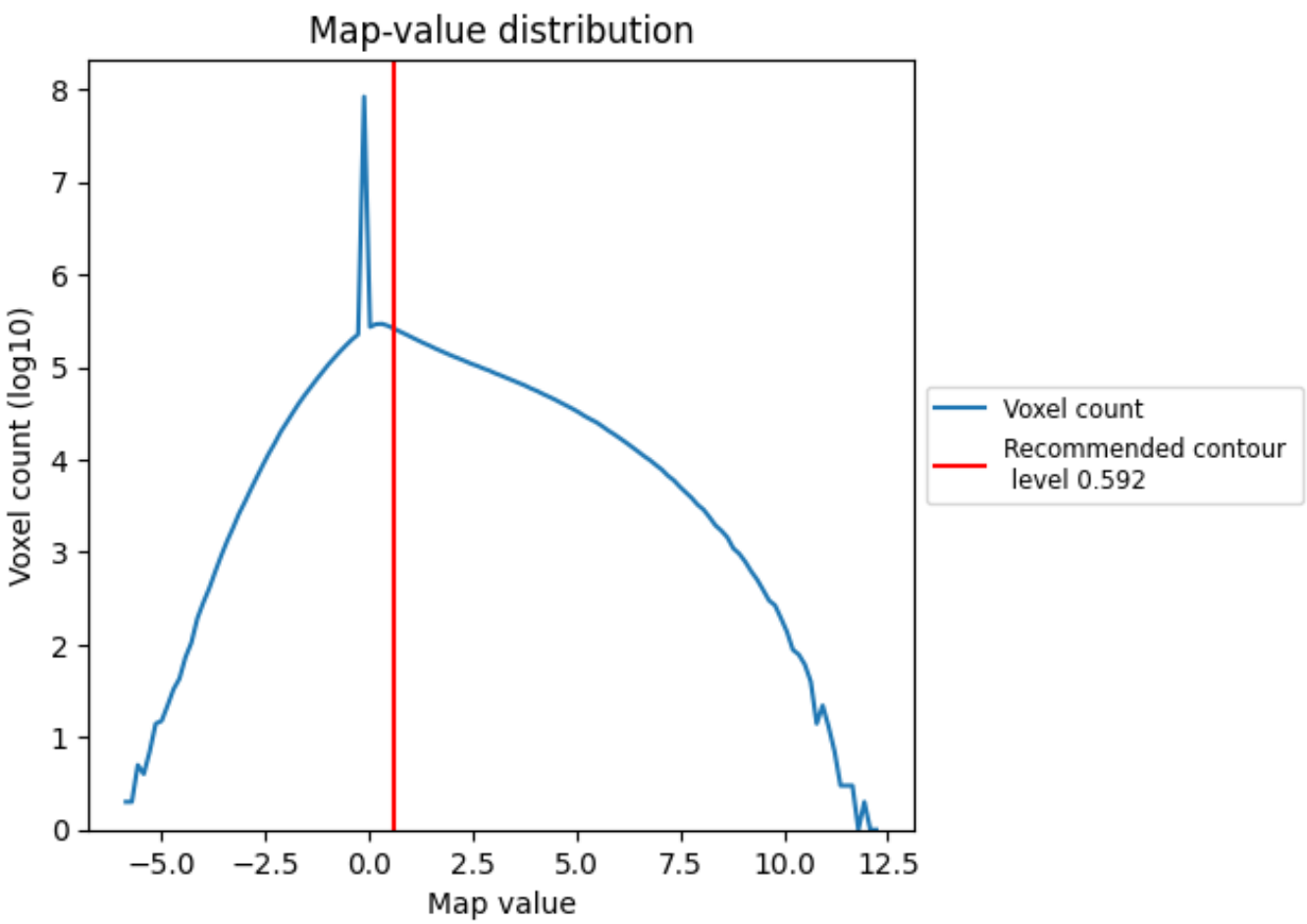
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

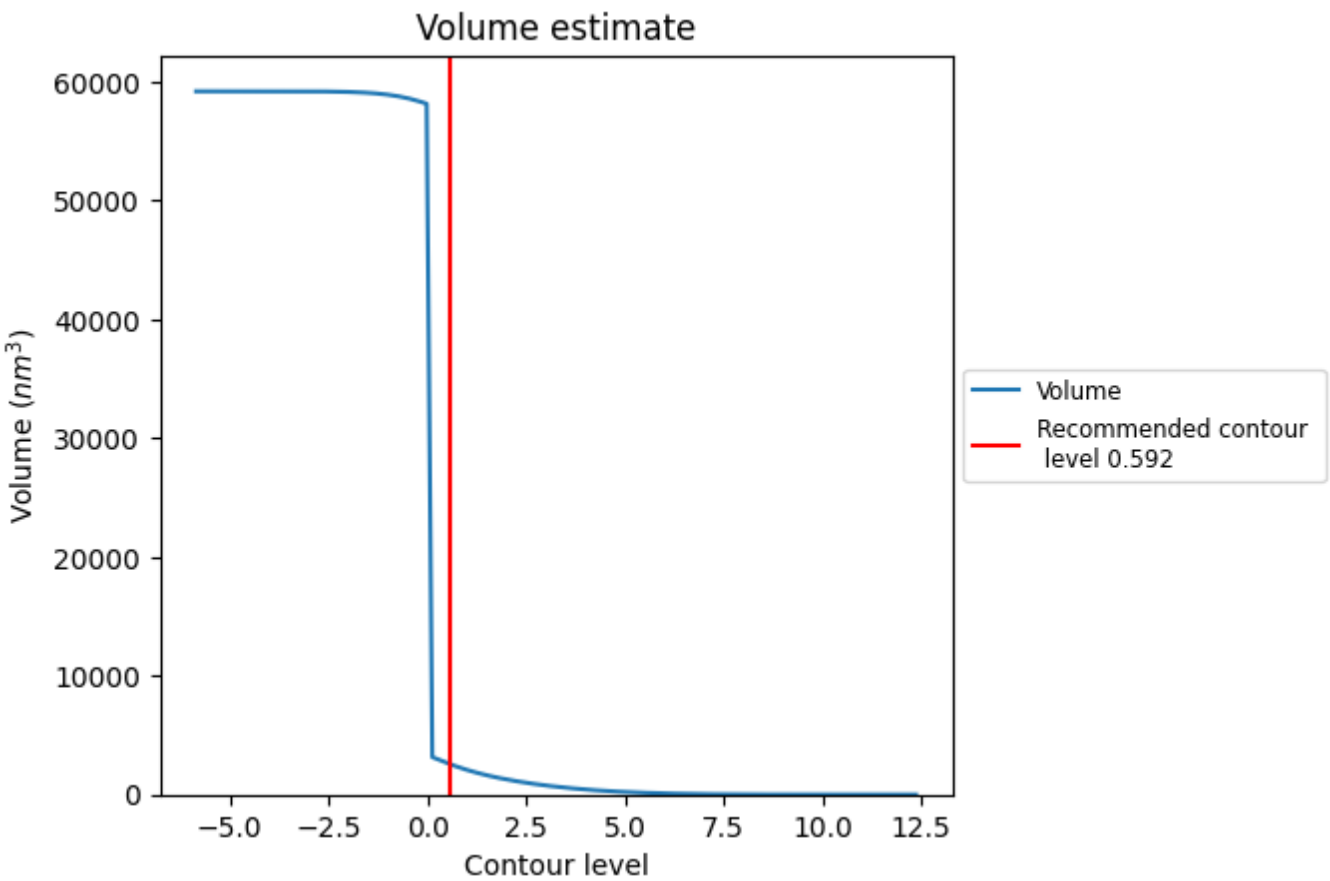
This section contains the results of statistical analysis of the map.

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.

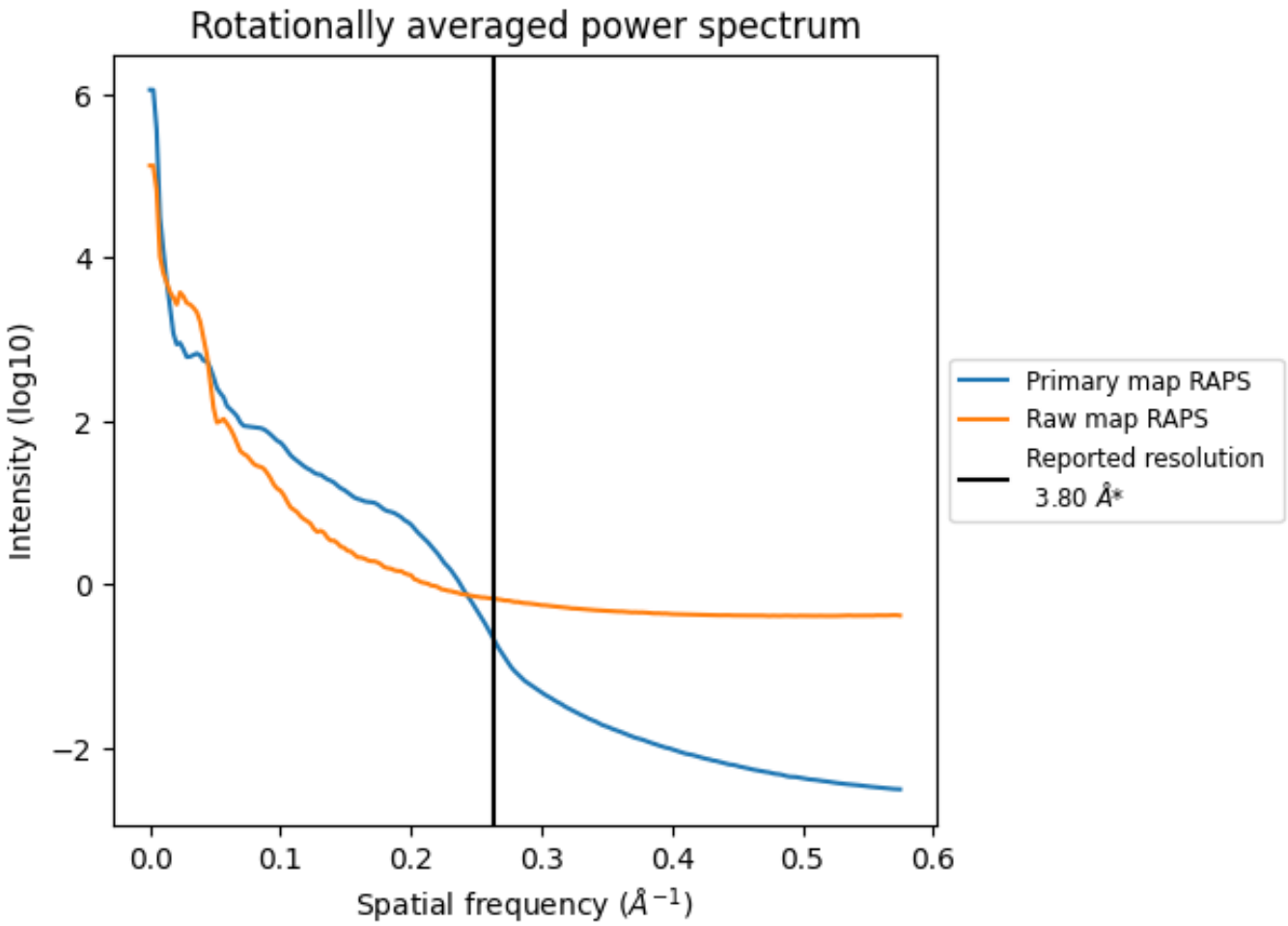
7.2 Volume estimate (i)



The volume at the recommended contour level is 2536 nm^3; this corresponds to an approximate mass of 2291 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

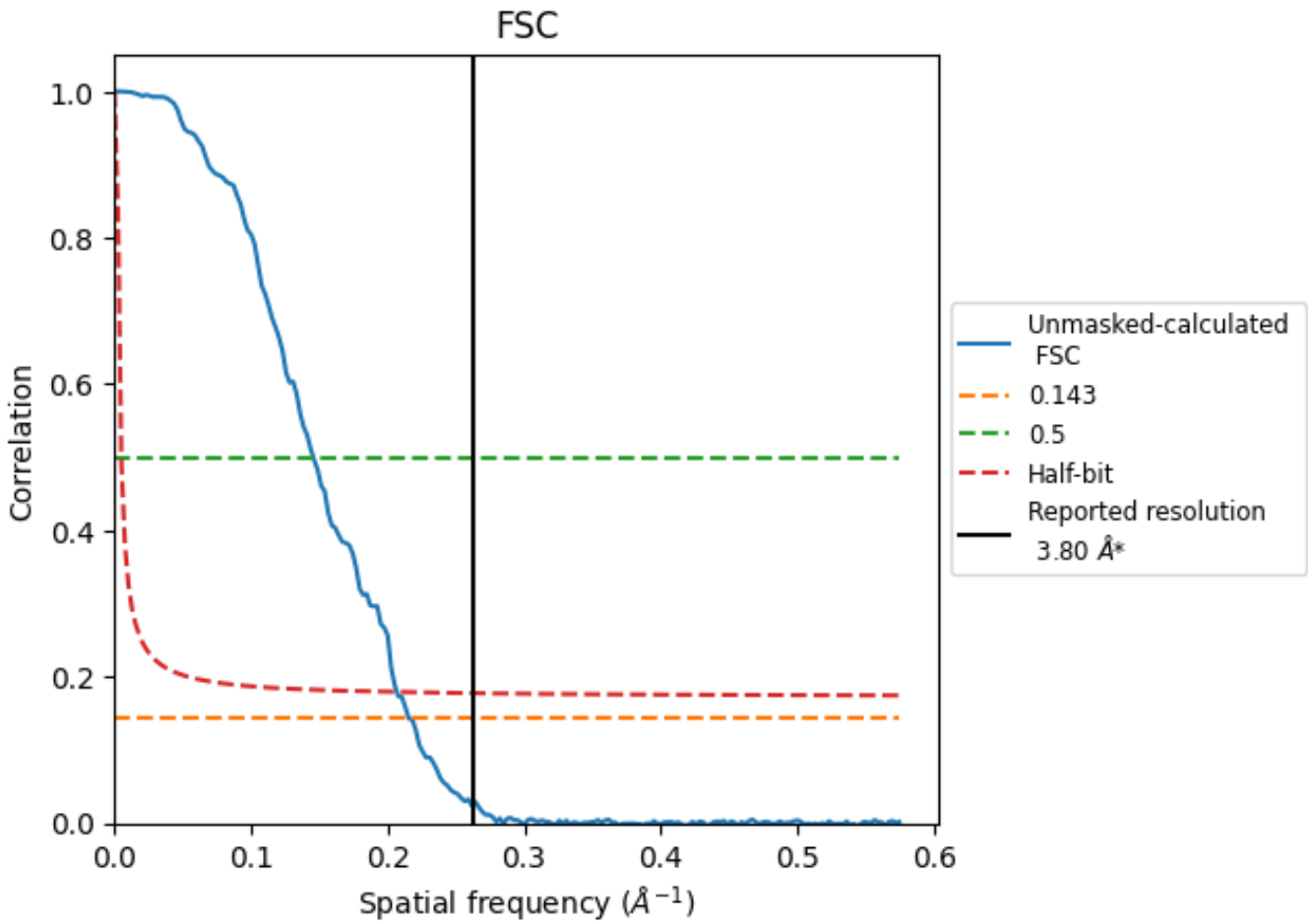


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

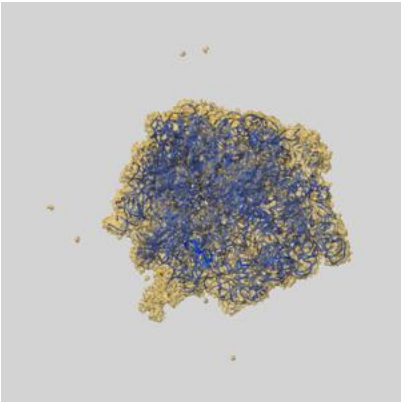
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.64	6.87	4.84

*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 4.64 differs from the reported value 3.8 by more than 10 %

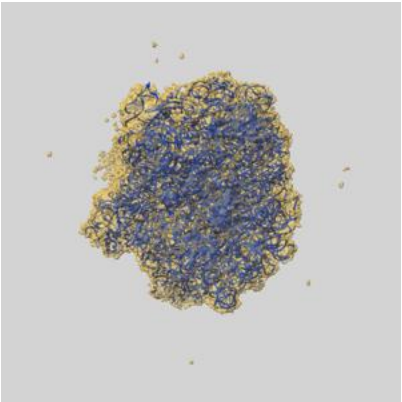
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22461 and PDB model 7JSW. Per-residue inclusion information can be found in section 3 on page 14.

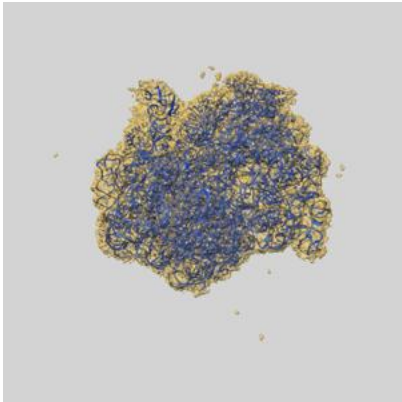
9.1 Map-model overlay (i)



X



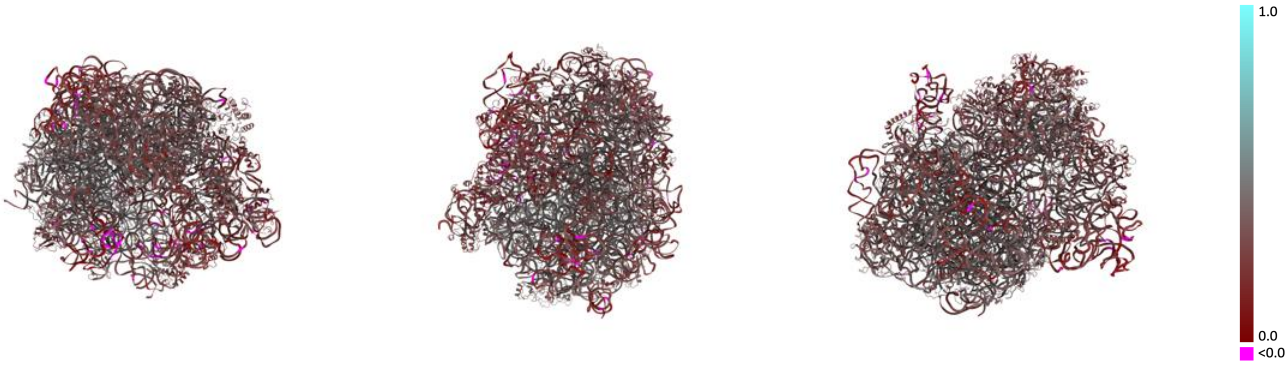
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.592 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.

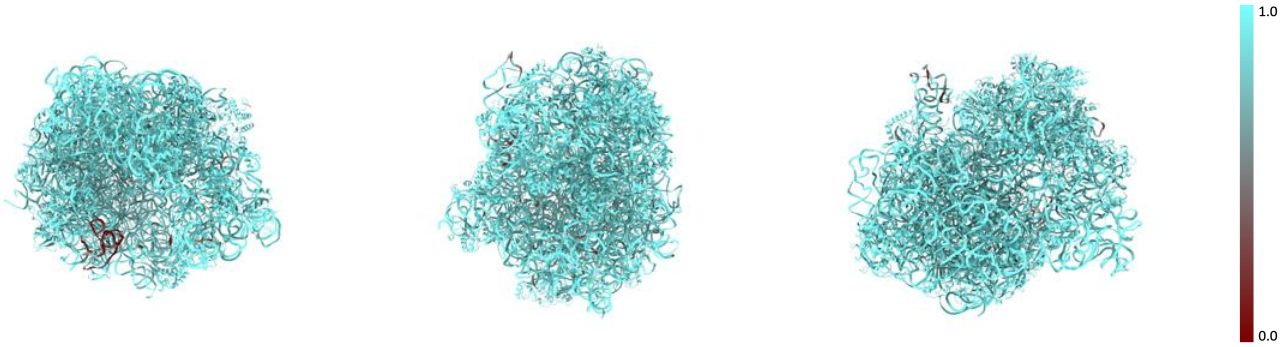
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

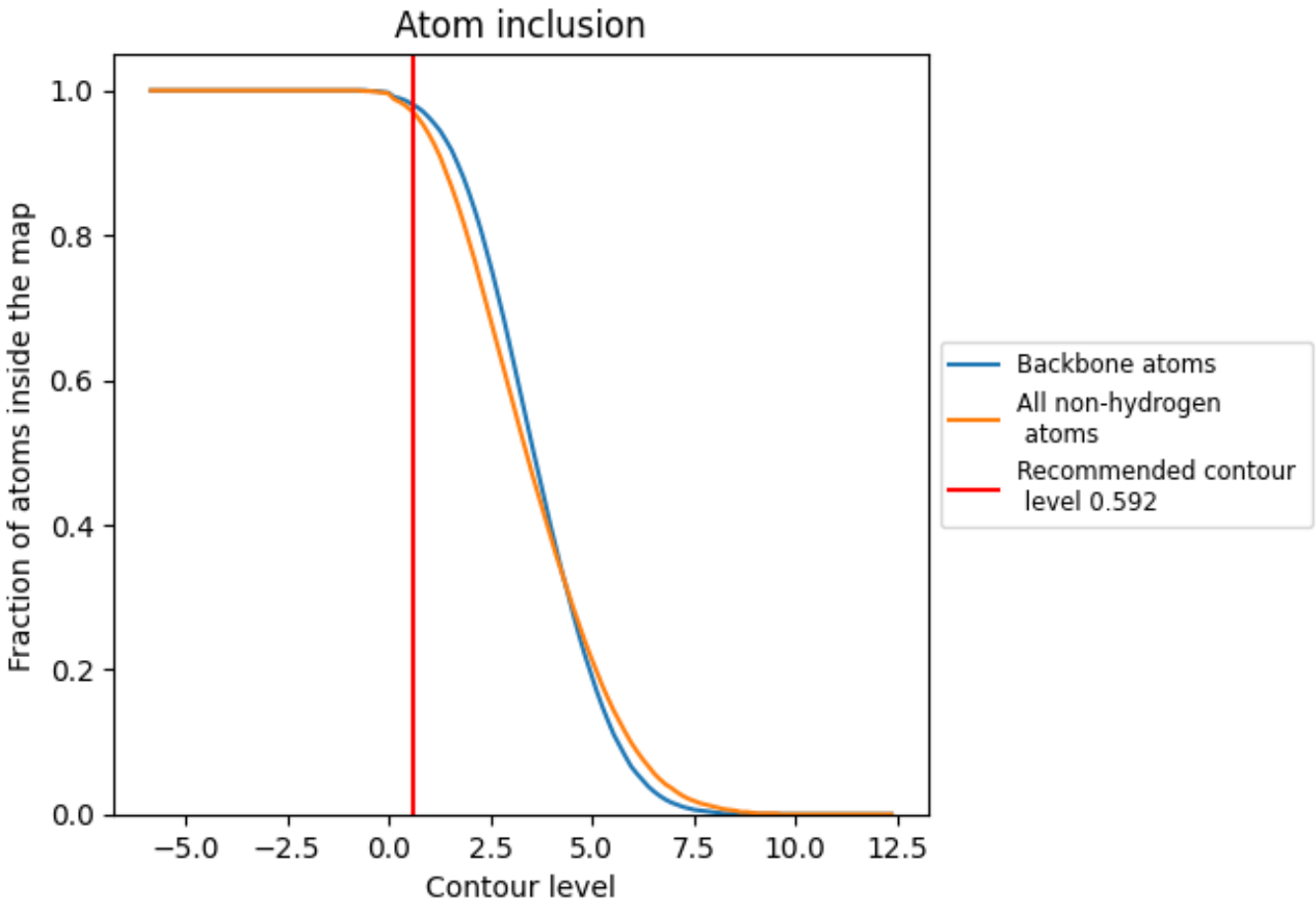
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.592).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.592) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9700	0.3390
1	0.9710	0.3530
2	0.9900	0.2920
3	0.9860	0.3110
4	0.9800	0.2840
5	0.9400	0.2280
8	0.7990	0.2150
B	0.9600	0.4140
C	0.9750	0.3980
D	0.9520	0.4270
E	0.9250	0.4070
F	0.9620	0.3810
G	0.9650	0.3040
H	0.9510	0.3320
I	0.9450	0.2990
J	0.9710	0.3650
K	0.9760	0.3140
L	0.9430	0.2640
M	0.9650	0.3440
N	0.9440	0.2610
O	0.9230	0.2810
P	0.9680	0.3250
Q	0.9700	0.3950
R	0.9770	0.2660
S	0.9680	0.2920
T	0.9680	0.3180
U	0.9540	0.3300
V	0.9750	0.3510
W	0.9130	0.3130
X	0.9940	0.2500
Y	0.9710	0.3090
Z	0.9030	0.2660
b	0.9550	0.4150
c	0.9610	0.4160
d	0.9690	0.3780

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Chain	Atom inclusion	Q-score
e	0.9690	0.2420
f	0.9750	0.3050
g	0.9080	0.2760
j	0.9580	0.3970
k	0.9660	0.4170
l	0.9670	0.4100
m	0.9660	0.4040
n	0.9770	0.4130
o	0.9840	0.3270
p	0.9810	0.3980
q	0.9580	0.4000
r	0.9750	0.4040
s	0.9550	0.4130
t	0.9680	0.3930
u	0.9670	0.3670
v	0.9800	0.3630
w	0.9480	0.4080
x	0.9800	0.3980
y	0.9780	0.3320
z	0.9700	0.4070