



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 01:28 PM EST

PDB ID : 6WNT
EMDB ID : EMD-21856
Title : 50S ribosomal subunit without free 5S rRNA and perturbed PTC
Authors : Loveland, A.B.; Korostelev, A.A.; Mankin, A.S.; Huang, S.; Aleksashin, N.A.; Klepacki, D.; Reier, K.; Kefi, A.; Szal, A.; Remme, J.; Jaeger, L.; Vazquez-Laslop, N.
Deposited on : 2020-04-23
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

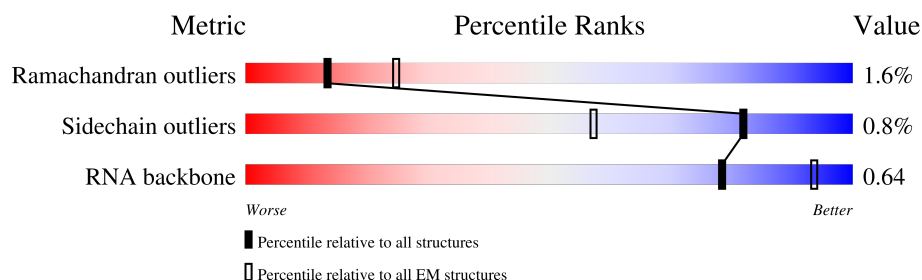
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



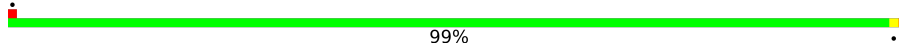
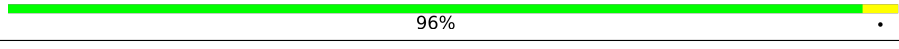
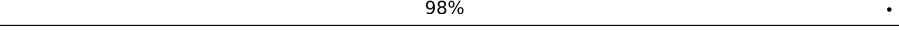
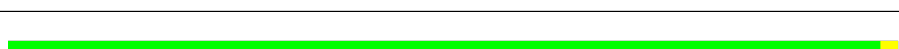
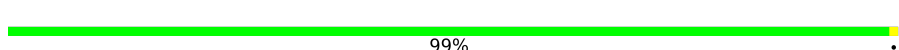
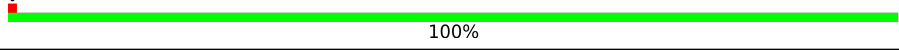
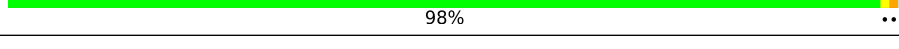
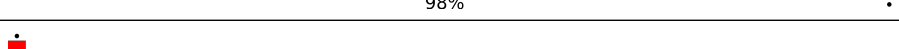

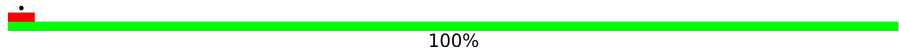
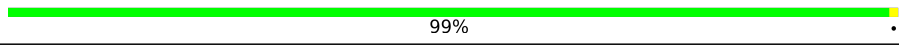
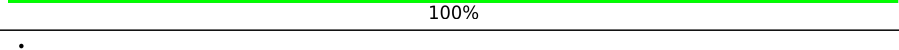
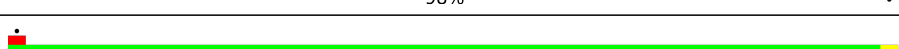
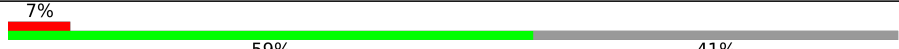
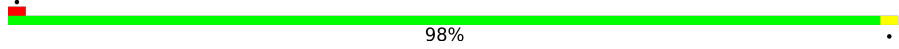
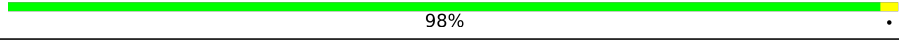
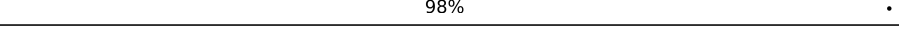






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. 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	b	271	
2	c	209	
3	d	201	
4	e	177	
5	f	176	
6	g	149	
7	h	131	
8	i	141	

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Mol	Chain	Length	Quality of chain
9	j	142	
10	k	122	
11	l	143	
12	n	120	
13	o	116	
14	p	114	
15	q	117	
16	r	103	
17	s	110	
18	t	93	
19	u	102	
20	v	94	
21	w	75	
22	x	77	
23	y	63	
24	z	58	
25	A	70	
26	B	56	
27	D	46	
28	E	64	
29	F	38	
30	a	223	
31	4	3031	

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 91164 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
1	b	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	209	Total	C	N	O	S	0	0
			1564	979	288	293	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	201	Total	C	N	O	S	0	0
			1551	974	283	289	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	176	Total	C	N	O	S	0	0
			1322	832	243	245	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	53	Total	C	N	O	S	0	0
			409	261	74	73	1		

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	141	Total	C	N	O	S	0	0
			1031	651	179	195	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	142	Total	C	N	O	S	0	0
			1128	714	212	198	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	l	143	Total	C	N	O	S	0	0
			1044	649	206	188	1		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	o	116	Total	C	N	O	0	0
			891	552	178	161		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	p	114	Total	C	N	O	S	0	0
			916	574	179	162	1		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	q	117	Total	C	N	O	S	0	0
			946	604	192	150			

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	r	103	Total	C	N	O	S	0	0
			815	516	153	144	2		

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	s	110	Total	C	N	O	S	0	0
			856	532	166	155	3		

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	t	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	u	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	v	94	Total	C	N	O	S	0	0
			752	479	137	133	3		

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	w	75	Total	C	N	O	S	0	0
			574	356	116	101	1		

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	x	77	Total	C	N	O	S	0	0
			624	388	129	105	2		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	y	63	Total	C	N	O	S	0	0
			508	313	99	94	2		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	41	Total	C	N	O	S	0	0
			315	192	57	60	6		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	56	Total	C	N	O	S	0	0
			443	269	94	79	1		

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D	46	Total	C	N	O	S	0	0
			376	228	90	56	2		

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	E	64	Total	C	N	O	S	0	0
			503	323	105	73	2		

- Molecule 29 is a protein called 50S ribosomal protein L36.

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

- Molecule 30 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 31 is a RNA chain called 23s-5s joint ribosomal RNA.

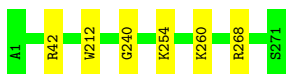
Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	3025	Total	C	N	O	P	0	0
			64925	28962	11938	21001	3024		

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.

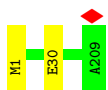
- Molecule 1: 50S ribosomal protein L2

Chain b:  98%



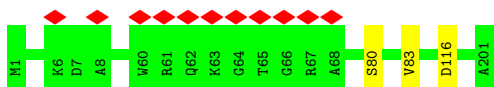
- Molecule 2: 50S ribosomal protein L3

Chain c:  99%



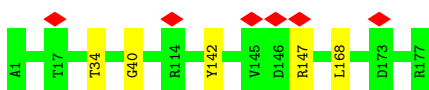
- Molecule 3: 50S ribosomal protein L4

Chain d:  5% 99%



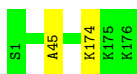
- Molecule 4: 50S ribosomal protein L5

Chain e:  97%



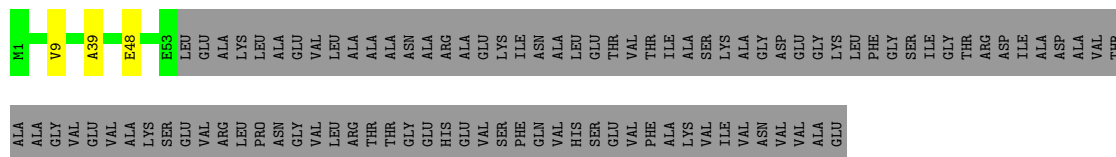
- Molecule 5: 50S ribosomal protein L6

Chain f:  99%



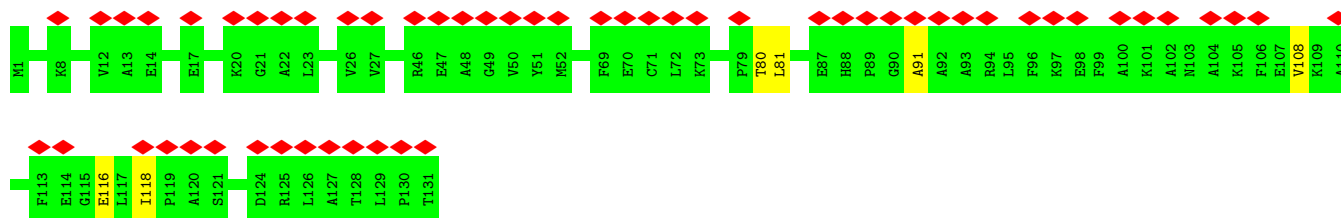
- Molecule 6: 50S ribosomal protein L9

Chain g:  34% 64%

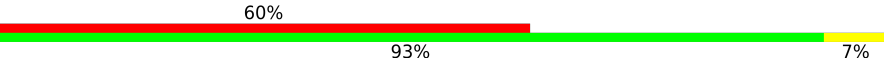


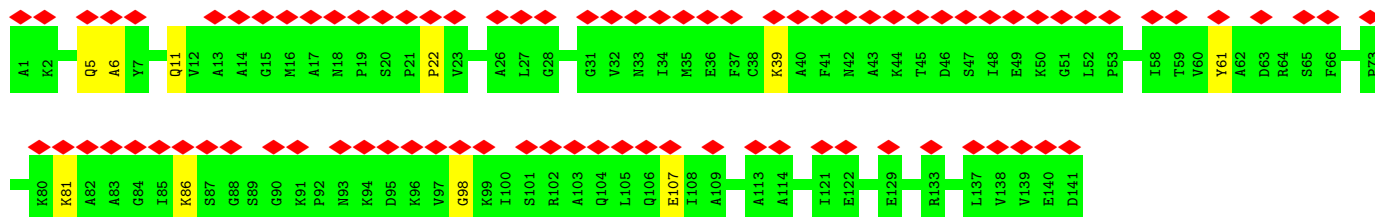
• Molecule 7: 50S ribosomal protein L10

Chain h:  43% 95% 5%



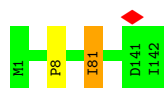
• Molecule 8: 50S ribosomal protein L11

Chain i:  60% 93% 7%



• Molecule 9: 50S ribosomal protein L13

Chain j:  99% 2%



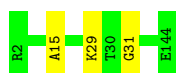
• Molecule 10: 50S ribosomal protein L14

Chain k:  96% 4%



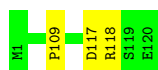
• Molecule 11: 50S ribosomal protein L15

Chain l:  98% 2%



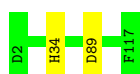
- Molecule 12: 50S ribosomal protein L17

Chain n: 98% .



- Molecule 13: 50S ribosomal protein L18

Chain o: 98% .



- Molecule 14: 50S ribosomal protein L19

Chain p: 99% .



- Molecule 15: 50S ribosomal protein L20

Chain q: 100% .



- Molecule 16: 50S ribosomal protein L21

Chain r: 98% ..



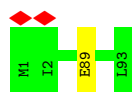
- Molecule 17: 50S ribosomal protein L22

Chain s: 98% .

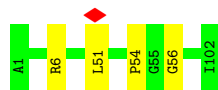


- Molecule 18: 50S ribosomal protein L23

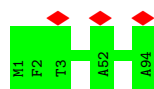
Chain t: 99% .



- Molecule 19: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L27

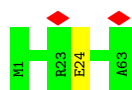


- Molecule 22: 50S ribosomal protein L28



There are no outlier residues recorded for this chain.

- Molecule 23: 50S ribosomal protein L29

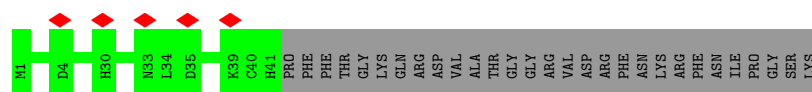


- Molecule 24: 50S ribosomal protein L30

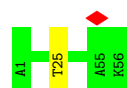


- Molecule 25: 50S ribosomal protein L31





- Molecule 26: 50S ribosomal protein L32



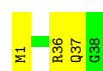
- Molecule 27: 50S ribosomal protein L34



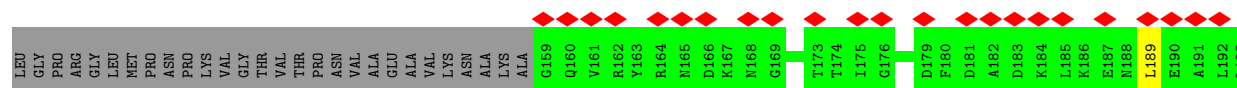
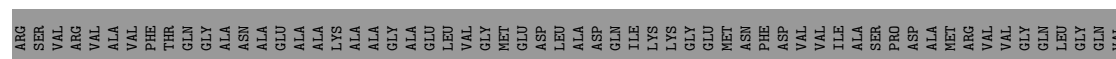
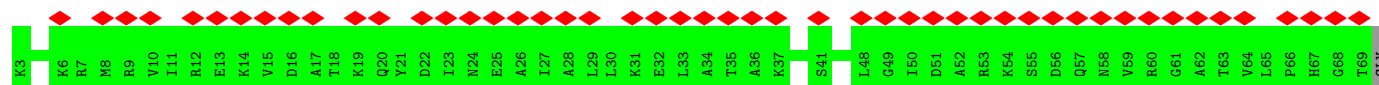
- Molecule 28: 50S ribosomal protein L35




- Molecule 29: 50S ribosomal protein L36

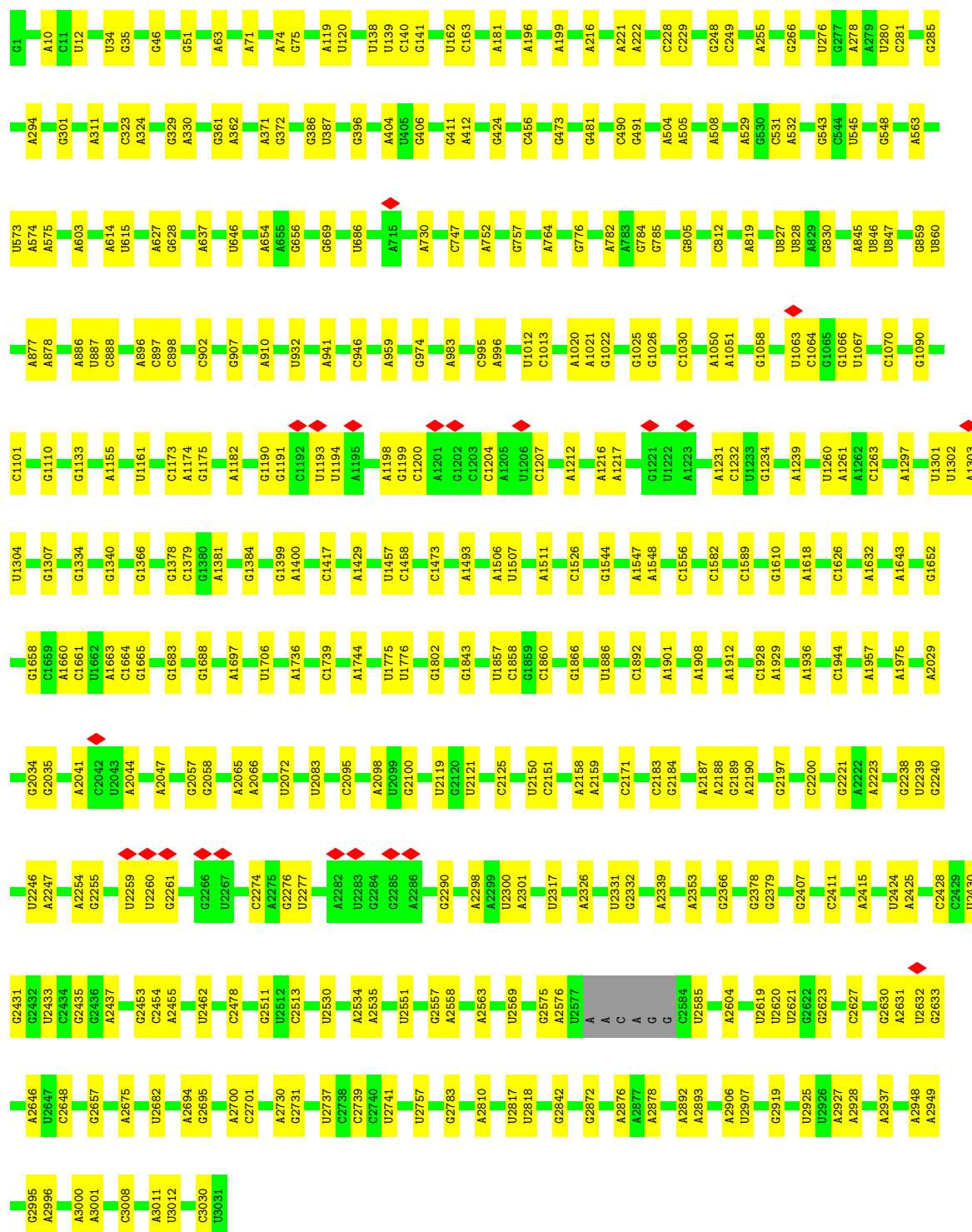


- Molecule 30: 50S ribosomal protein L1



- Molecule 31: 23s-5s joint ribosomal RNA

Chain 4:  87% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21705	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	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	19.138	Depositor
Minimum map value	-6.456	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.774	Depositor
Recommended contour level	2.5	Depositor
Map size (\AA)	528.96, 528.96, 528.96	wwPDB
Map dimensions	608, 608, 608	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.87000006, 0.87000006, 0.87000006	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	0.33	0/2121	0.58	0/2852
2	c	0.33	0/1585	0.56	0/2134
3	d	0.36	0/1570	0.54	0/2113
4	e	0.43	0/1434	0.56	0/1926
5	f	0.34	0/1342	0.53	0/1816
6	g	0.40	0/414	0.63	0/556
7	h	0.47	0/1001	0.68	0/1350
8	i	0.45	0/1045	0.61	0/1410
9	j	0.31	0/1151	0.52	0/1551
10	k	0.33	0/947	0.58	0/1268
11	l	0.34	0/1053	0.58	0/1403
12	n	0.32	0/973	0.54	0/1301
13	o	0.33	0/901	0.52	0/1209
14	p	0.33	0/928	0.55	0/1242
15	q	0.34	0/959	0.48	0/1278
16	r	0.37	0/828	0.61	0/1107
17	s	0.29	0/863	0.54	0/1156
18	t	0.32	0/744	0.53	0/994
19	u	0.35	0/787	0.57	0/1051
20	v	0.38	0/765	0.53	0/1025
21	w	0.36	0/581	0.52	0/769
22	x	0.33	0/634	0.56	0/848
23	y	0.33	0/509	0.50	0/677
24	z	0.28	0/452	0.50	0/605
25	A	0.35	0/319	0.55	0/426
26	B	0.30	0/449	0.55	0/599
27	D	0.34	0/379	0.55	0/498
28	E	0.33	0/512	0.56	0/676
29	F	0.27	0/303	0.58	0/397
30	a	0.42	0/1033	0.57	0/1387
31	4	0.40	0/72710	0.66	0/113431
All	All	0.39	0/99292	0.64	0/149055

There are no bond length outliers.

There are no bond angle outliers.

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%)	237 (88%)	29 (11%)	3 (1%)	14	46
2	c	207/209 (99%)	187 (90%)	19 (9%)	1 (0%)	29	64
3	d	199/201 (99%)	177 (89%)	20 (10%)	2 (1%)	15	49
4	e	175/177 (99%)	150 (86%)	23 (13%)	2 (1%)	14	46
5	f	174/176 (99%)	157 (90%)	15 (9%)	2 (1%)	14	46
6	g	51/149 (34%)	37 (72%)	11 (22%)	3 (6%)	1	10
7	h	129/131 (98%)	97 (75%)	26 (20%)	6 (5%)	2	14
8	i	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	3	20
9	j	140/142 (99%)	131 (94%)	7 (5%)	2 (1%)	11	40
10	k	120/122 (98%)	99 (82%)	18 (15%)	3 (2%)	5	27
11	l	141/143 (99%)	122 (86%)	16 (11%)	3 (2%)	7	30
12	n	118/120 (98%)	104 (88%)	11 (9%)	3 (2%)	5	27
13	o	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	17	52
14	p	112/114 (98%)	96 (86%)	15 (13%)	1 (1%)	17	52
15	q	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
16	r	101/103 (98%)	88 (87%)	11 (11%)	2 (2%)	7	31
17	s	108/110 (98%)	98 (91%)	8 (7%)	2 (2%)	8	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	t	91/93 (98%)	82 (90%)	8 (9%)	1 (1%)	14	46
19	u	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	3	17
20	v	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
21	w	73/75 (97%)	65 (89%)	7 (10%)	1 (1%)	11	40
22	x	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
23	y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	9	37
24	z	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
25	A	39/70 (56%)	35 (90%)	4 (10%)	0	100	100
26	B	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	8	33
27	D	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
28	E	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	9	37
29	F	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	25
30	a	130/223 (58%)	114 (88%)	14 (11%)	2 (2%)	10	39
All	All	3325/3601 (92%)	2925 (88%)	347 (10%)	53 (2%)	13	37

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	c	30	GLU
3	d	83	VAL
5	f	174	LYS
6	g	9	VAL
7	h	80	THR
7	h	108	VAL
9	j	81	ILE
10	k	89	ASN
11	l	31	GLY
16	r	54	VAL
19	u	6	ARG
21	w	12	SER
23	y	24	GLU
26	B	25	THR
29	F	37	GLN
30	a	217	THR
7	h	81	LEU
8	i	5	GLN
8	i	6	ALA

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Mol	Chain	Res	Type
8	i	11	GLN
8	i	98	GLY
12	n	118	ARG
19	u	56	GLY
30	a	202	THR
11	l	15	ALA
11	l	29	LYS
19	u	54	PRO
4	e	142	TYR
7	h	91	ALA
7	h	118	ILE
10	k	92	GLU
16	r	52	PRO
17	s	3	THR
19	u	51	LEU
1	b	254	LYS
1	b	260	LYS
3	d	80	SER
6	g	48	GLU
7	h	116	GLU
8	i	22	PRO
10	k	93	GLN
12	n	117	ASP
13	o	34	HIS
17	s	74	ILE
18	t	89	GLU
5	f	45	ALA
6	g	39	ALA
14	p	64	SER
28	E	31	ILE
9	j	8	PRO
12	n	109	PRO
1	b	240	GLY
4	e	40	GLY

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	b	216/216 (100%)	213 (99%)	3 (1%)	67	86
2	c	164/164 (100%)	163 (99%)	1 (1%)	86	94
3	d	165/165 (100%)	164 (99%)	1 (1%)	86	94
4	e	148/148 (100%)	145 (98%)	3 (2%)	55	80
5	f	137/137 (100%)	137 (100%)	0	100	100
6	g	42/114 (37%)	42 (100%)	0	100	100
7	h	100/100 (100%)	100 (100%)	0	100	100
8	i	109/109 (100%)	104 (95%)	5 (5%)	27	59
9	j	116/116 (100%)	115 (99%)	1 (1%)	78	91
10	k	103/103 (100%)	101 (98%)	2 (2%)	57	81
11	l	102/102 (100%)	102 (100%)	0	100	100
12	n	100/100 (100%)	100 (100%)	0	100	100
13	o	86/86 (100%)	85 (99%)	1 (1%)	71	88
14	p	99/99 (100%)	99 (100%)	0	100	100
15	q	89/89 (100%)	89 (100%)	0	100	100
16	r	84/84 (100%)	83 (99%)	1 (1%)	71	88
17	s	93/93 (100%)	93 (100%)	0	100	100
18	t	80/80 (100%)	80 (100%)	0	100	100
19	u	83/83 (100%)	83 (100%)	0	100	100
20	v	78/78 (100%)	78 (100%)	0	100	100
21	w	57/57 (100%)	57 (100%)	0	100	100
22	x	67/67 (100%)	67 (100%)	0	100	100
23	y	55/55 (100%)	55 (100%)	0	100	100
24	z	48/48 (100%)	47 (98%)	1 (2%)	53	79
25	A	38/62 (61%)	38 (100%)	0	100	100
26	B	47/47 (100%)	47 (100%)	0	100	100
27	D	38/38 (100%)	37 (97%)	1 (3%)	46	74
28	E	51/51 (100%)	51 (100%)	0	100	100
29	F	34/34 (100%)	32 (94%)	2 (6%)	19	50
30	a	110/174 (63%)	109 (99%)	1 (1%)	78	91
All	All	2739/2899 (94%)	2716 (99%)	23 (1%)	82	92

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	42	ARG
1	b	212	TRP
1	b	268	ARG
2	c	1	MET
3	d	116	ASP
4	e	34	THR
4	e	147	ARG
4	e	168	LEU
8	i	39	LYS
8	i	61	TYR
8	i	81	LYS
8	i	86	LYS
8	i	107	GLU
9	j	81	ILE
10	k	31	ARG
10	k	58	LEU
13	o	89	ASP
16	r	54	VAL
24	z	30	ARG
27	D	44	VAL
29	F	1	MET
29	F	36	ARG
30	a	189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	127	ASN
1	b	238	ASN
1	b	250	GLN
1	b	259	ASN
2	c	49	GLN
2	c	164	GLN
2	c	173	GLN
3	d	41	GLN
3	d	97	ASN
4	e	80	GLN
5	f	115	GLN
5	f	138	GLN
7	h	122	GLN
8	i	33	ASN
9	j	58	ASN
9	j	80	HIS

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Mol	Chain	Res	Type
10	k	3	GLN
11	l	38	GLN
12	n	3	HIS
13	o	29	HIS
13	o	100	HIS
14	p	11	GLN
14	p	114	ASN
15	q	36	GLN
15	q	58	GLN
16	r	6	GLN
17	s	7	HIS
18	t	15	HIS
18	t	59	ASN
18	t	70	HIS
19	u	39	ASN
19	u	68	ASN
19	u	73	ASN
20	v	12	GLN
20	v	24	ASN
20	v	87	GLN
21	w	53	HIS
22	x	15	ASN
22	x	16	ASN
22	x	22	ASN
23	y	20	ASN
23	y	36	GLN
23	y	41	HIS
24	z	19	HIS
25	A	20	ASN
25	A	41	HIS
26	B	3	GLN
26	B	4	GLN
26	B	5	ASN
28	E	30	HIS
28	E	42	HIS
29	F	35	GLN
29	F	37	GLN
30	a	20	GLN
30	a	47	ASN
30	a	57	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	4	3023/3031 (99%)	370 (12%)	9 (0%)

All (370) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
31	4	10	A
31	4	12	U
31	4	34	U
31	4	35	G
31	4	46	G
31	4	51	G
31	4	63	A
31	4	71	A
31	4	74	A
31	4	75	G
31	4	119	A
31	4	120	U
31	4	138	U
31	4	139	U
31	4	140	C
31	4	141	G
31	4	162	U
31	4	163	C
31	4	181	A
31	4	196	A
31	4	199	A
31	4	216	A
31	4	221	A
31	4	222	A
31	4	228	C
31	4	229	C
31	4	248	G
31	4	249	C
31	4	255	A
31	4	266	G
31	4	276	U
31	4	278	A
31	4	280	U
31	4	281	C
31	4	285	G
31	4	294	A
31	4	301	G
31	4	311	A

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Mol	Chain	Res	Type
31	4	323	C
31	4	324	A
31	4	329	G
31	4	330	A
31	4	361	G
31	4	362	A
31	4	371	A
31	4	372	G
31	4	386	G
31	4	387	U
31	4	396	G
31	4	404	A
31	4	406	G
31	4	411	G
31	4	412	A
31	4	424	G
31	4	456	C
31	4	473	G
31	4	481	G
31	4	491	G
31	4	504	A
31	4	505	A
31	4	508	A
31	4	529	A
31	4	531	C
31	4	532	A
31	4	543	G
31	4	545	U
31	4	548	G
31	4	563	A
31	4	573	U
31	4	574	A
31	4	575	A
31	4	603	A
31	4	614	A
31	4	615	U
31	4	627	A
31	4	628	G
31	4	637	A
31	4	646	U
31	4	654	A
31	4	656	G

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Mol	Chain	Res	Type
31	4	669	G
31	4	686	U
31	4	730	A
31	4	747	C
31	4	752	A
31	4	757	G
31	4	764	A
31	4	776	G
31	4	782	A
31	4	784	G
31	4	785	G
31	4	805	G
31	4	812	C
31	4	819	A
31	4	827	U
31	4	828	U
31	4	830	G
31	4	845	A
31	4	846	U
31	4	847	U
31	4	860	U
31	4	877	A
31	4	878	A
31	4	886	A
31	4	887	U
31	4	888	C
31	4	896	A
31	4	897	C
31	4	898	C
31	4	902	C
31	4	907	G
31	4	910	A
31	4	932	U
31	4	941	A
31	4	946	C
31	4	959	A
31	4	974	G
31	4	983	A
31	4	995	C
31	4	996	A
31	4	1012	U
31	4	1013	C

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Mol	Chain	Res	Type
31	4	1021	A
31	4	1022	G
31	4	1025	G
31	4	1026	G
31	4	1030	C
31	4	1050	A
31	4	1051	A
31	4	1058	G
31	4	1063	U
31	4	1064	C
31	4	1066	G
31	4	1067	U
31	4	1070	C
31	4	1090	G
31	4	1101	C
31	4	1110	G
31	4	1133	G
31	4	1155	A
31	4	1161	U
31	4	1173	C
31	4	1174	A
31	4	1175	G
31	4	1182	A
31	4	1190	G
31	4	1191	G
31	4	1193	U
31	4	1194	U
31	4	1198	A
31	4	1199	G
31	4	1200	C
31	4	1204	C
31	4	1207	C
31	4	1212	A
31	4	1216	A
31	4	1217	A
31	4	1231	A
31	4	1232	C
31	4	1234	G
31	4	1239	A
31	4	1260	U
31	4	1261	A
31	4	1263	C

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Mol	Chain	Res	Type
31	4	1297	A
31	4	1301	U
31	4	1302	U
31	4	1303	A
31	4	1304	U
31	4	1307	G
31	4	1334	G
31	4	1340	G
31	4	1366	G
31	4	1378	G
31	4	1379	C
31	4	1381	A
31	4	1384	G
31	4	1399	G
31	4	1400	A
31	4	1417	C
31	4	1429	A
31	4	1457	U
31	4	1458	C
31	4	1473	C
31	4	1493	A
31	4	1506	A
31	4	1507	U
31	4	1511	A
31	4	1526	C
31	4	1544	G
31	4	1547	A
31	4	1548	A
31	4	1556	C
31	4	1582	C
31	4	1589	C
31	4	1610	G
31	4	1618	A
31	4	1626	C
31	4	1632	A
31	4	1643	A
31	4	1652	G
31	4	1658	G
31	4	1660	A
31	4	1661	C
31	4	1663	A
31	4	1664	C

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Mol	Chain	Res	Type
31	4	1665	G
31	4	1683	G
31	4	1688	G
31	4	1697	A
31	4	1706	U
31	4	1736	A
31	4	1739	C
31	4	1744	A
31	4	1775	U
31	4	1776	U
31	4	1802	G
31	4	1843	G
31	4	1857	U
31	4	1858	C
31	4	1860	C
31	4	1866	G
31	4	1886	U
31	4	1892	C
31	4	1901	A
31	4	1908	A
31	4	1912	A
31	4	1928	C
31	4	1929	A
31	4	1936	A
31	4	1944	C
31	4	1957	A
31	4	1975	A
31	4	2029	A
31	4	2034	G
31	4	2035	G
31	4	2041	A
31	4	2044	A
31	4	2047	A
31	4	2057	G
31	4	2058	G
31	4	2065	A
31	4	2066	A
31	4	2072	U
31	4	2083	U
31	4	2095	C
31	4	2098	A
31	4	2100	G

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Mol	Chain	Res	Type
31	4	2119	U
31	4	2121	U
31	4	2125	C
31	4	2150	U
31	4	2151	C
31	4	2158	A
31	4	2159	A
31	4	2171	C
31	4	2183	C
31	4	2184	G
31	4	2187	A
31	4	2188	A
31	4	2189	G
31	4	2190	A
31	4	2197	G
31	4	2200	C
31	4	2221	G
31	4	2223	A
31	4	2238	G
31	4	2239	U
31	4	2240	G
31	4	2246	U
31	4	2247	A
31	4	2254	A
31	4	2255	G
31	4	2259	U
31	4	2260	U
31	4	2261	G
31	4	2274	C
31	4	2276	G
31	4	2277	U
31	4	2290	G
31	4	2298	A
31	4	2300	U
31	4	2301	A
31	4	2317	U
31	4	2326	A
31	4	2331	U
31	4	2332	G
31	4	2339	A
31	4	2353	A
31	4	2366	G

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Mol	Chain	Res	Type
31	4	2378	G
31	4	2379	G
31	4	2407	G
31	4	2411	C
31	4	2415	A
31	4	2425	A
31	4	2428	C
31	4	2431	G
31	4	2433	U
31	4	2435	G
31	4	2437	A
31	4	2453	G
31	4	2455	A
31	4	2462	U
31	4	2478	C
31	4	2511	G
31	4	2513	C
31	4	2530	U
31	4	2534	A
31	4	2535	A
31	4	2551	U
31	4	2557	G
31	4	2558	A
31	4	2563	A
31	4	2569	U
31	4	2575	G
31	4	2576	A
31	4	2585	U
31	4	2604	A
31	4	2619	U
31	4	2620	U
31	4	2621	U
31	4	2623	G
31	4	2627	C
31	4	2630	G
31	4	2631	A
31	4	2632	U
31	4	2633	G
31	4	2646	A
31	4	2648	C
31	4	2657	G
31	4	2675	A

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Mol	Chain	Res	Type
31	4	2682	U
31	4	2694	A
31	4	2695	G
31	4	2700	A
31	4	2701	C
31	4	2730	A
31	4	2731	G
31	4	2737	U
31	4	2739	C
31	4	2741	U
31	4	2757	U
31	4	2783	G
31	4	2810	A
31	4	2817	U
31	4	2818	U
31	4	2842	G
31	4	2872	G
31	4	2876	A
31	4	2878	A
31	4	2892	A
31	4	2893	A
31	4	2906	A
31	4	2907	U
31	4	2919	G
31	4	2925	U
31	4	2927	A
31	4	2928	A
31	4	2937	A
31	4	2948	A
31	4	2949	A
31	4	2995	G
31	4	2996	A
31	4	3000	A
31	4	3001	A
31	4	3008	C
31	4	3011	A
31	4	3012	U
31	4	3030	C

All (9) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
31	4	490	C
31	4	859	G
31	4	1020	A
31	4	1025	G
31	4	2424	U
31	4	2430	U
31	4	2454	C
31	4	2632	U
31	4	3001	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

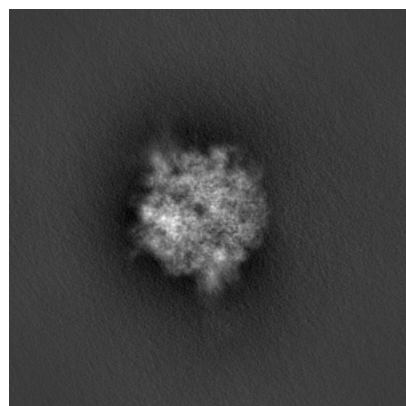
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21856. These allow visual inspection of the internal detail of the map and identification of artifacts.

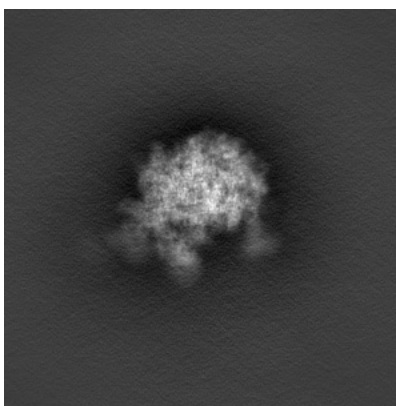
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

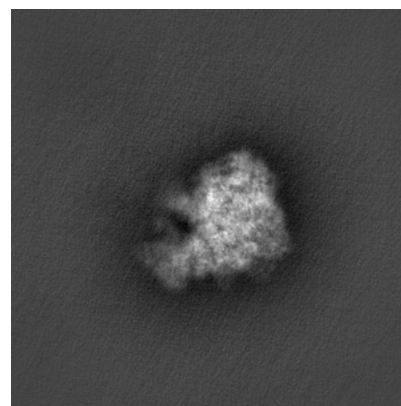
6.1.1 Primary map



X

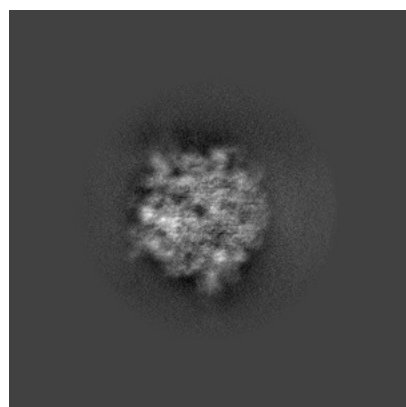


Y

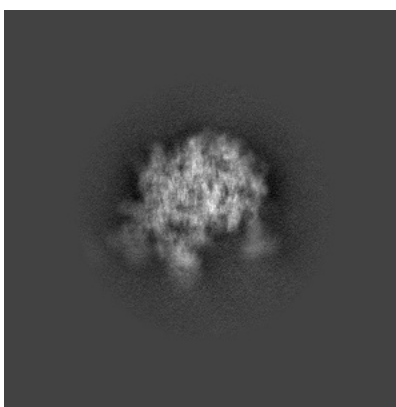


Z

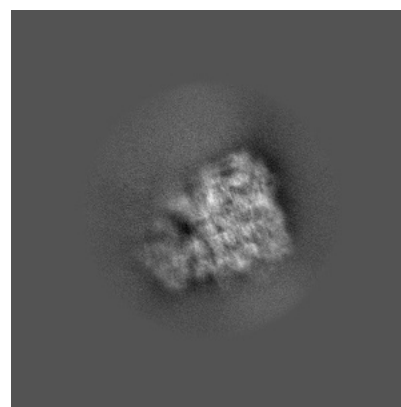
6.1.2 Raw map



X



Y

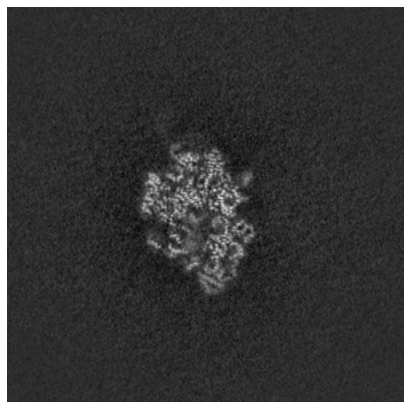


Z

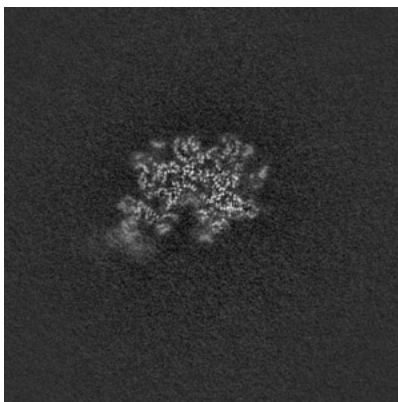
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

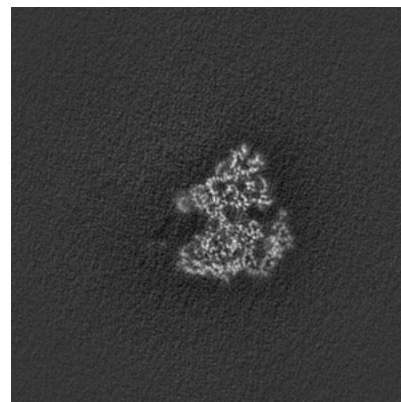
6.2.1 Primary map



X Index: 304

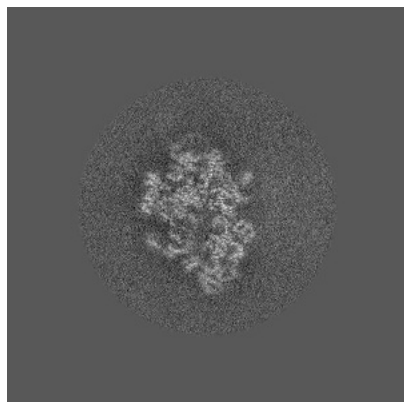


Y Index: 304

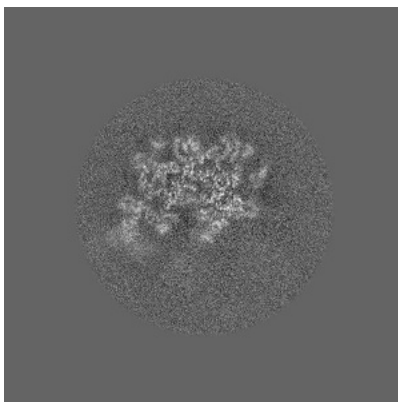


Z Index: 304

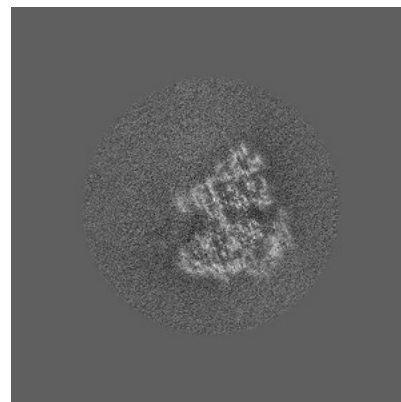
6.2.2 Raw map



X Index: 304



Y Index: 304

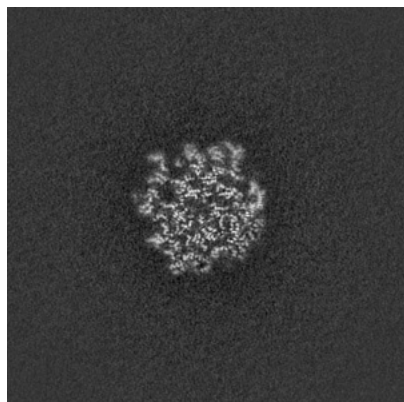


Z Index: 304

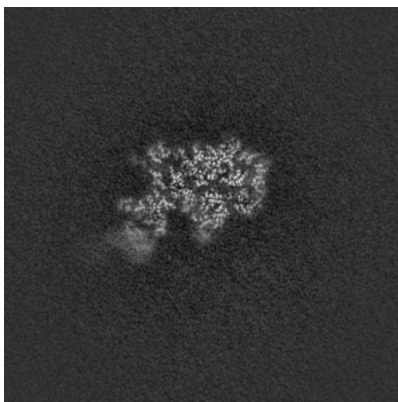
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

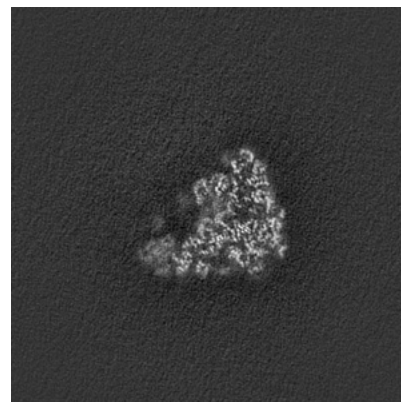
6.3.1 Primary map



X Index: 339

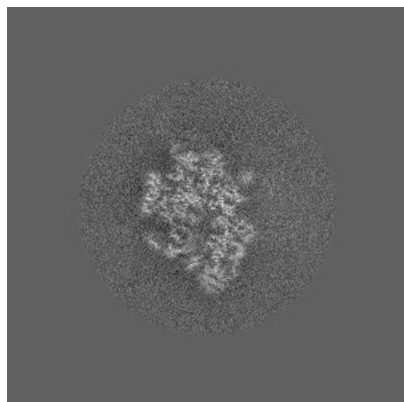


Y Index: 316

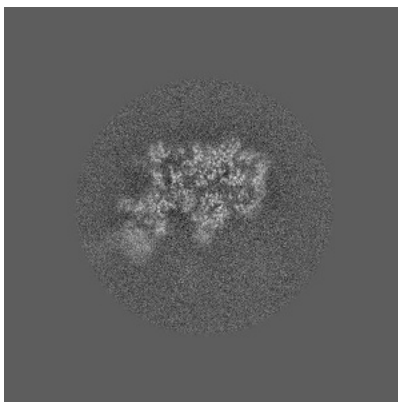


Z Index: 290

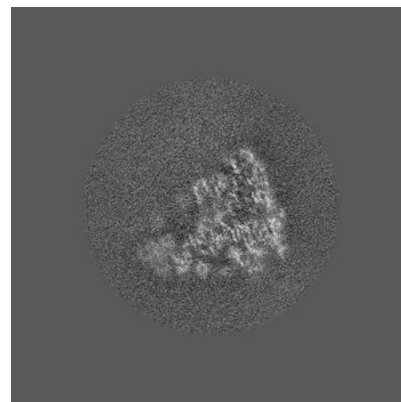
6.3.2 Raw map



X Index: 303



Y Index: 316

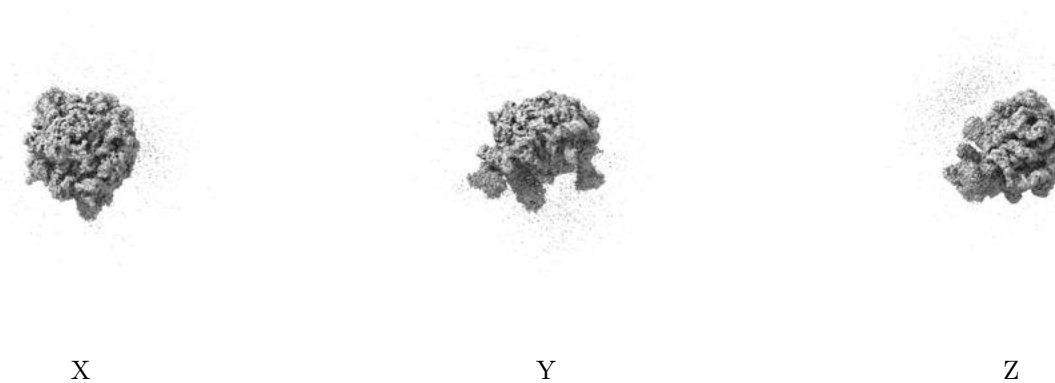


Z Index: 290

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

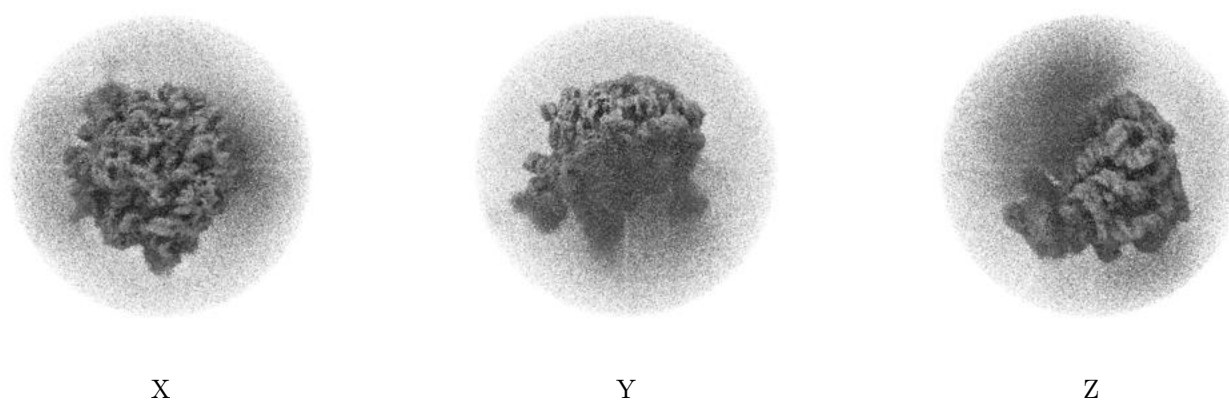
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

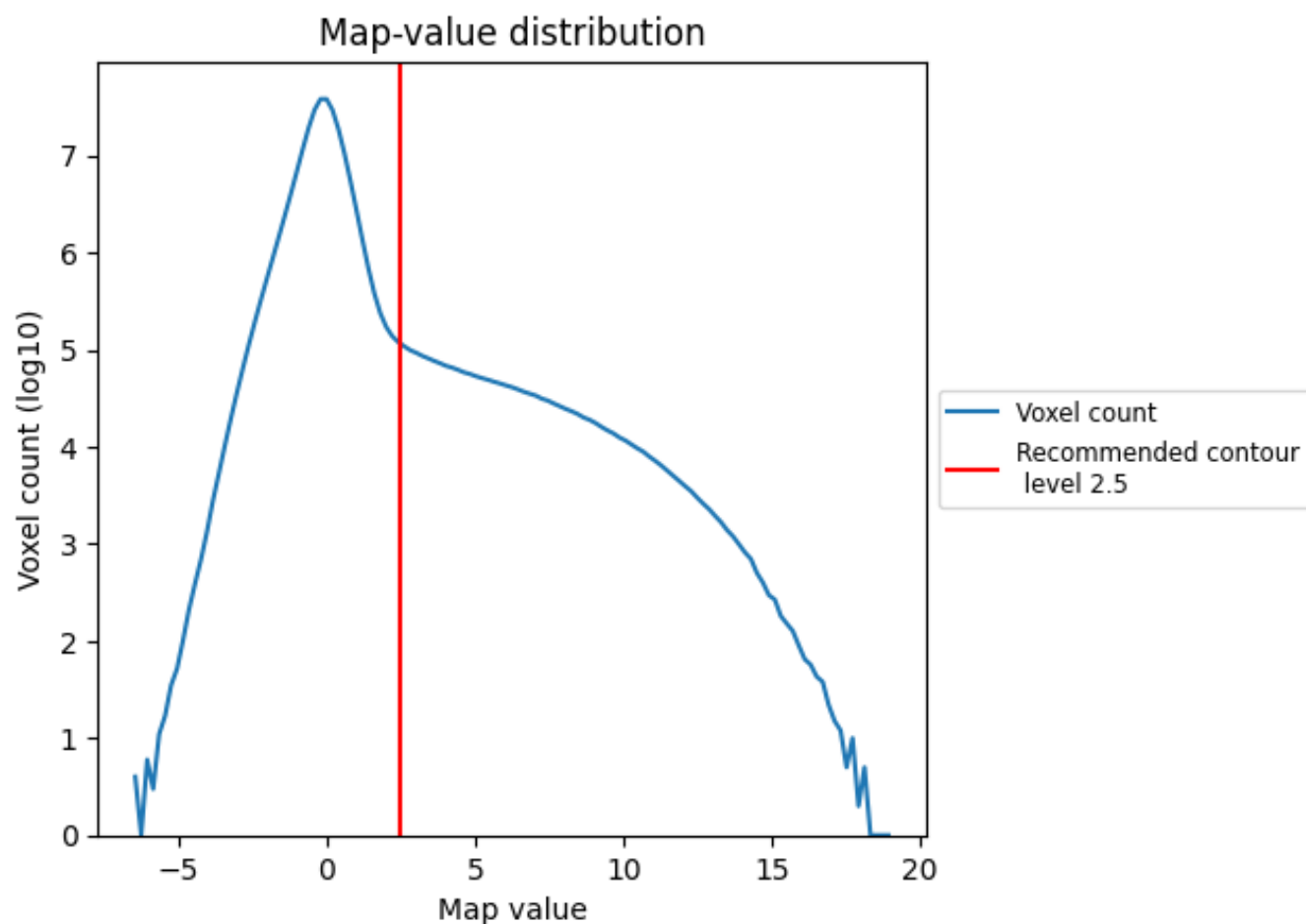
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

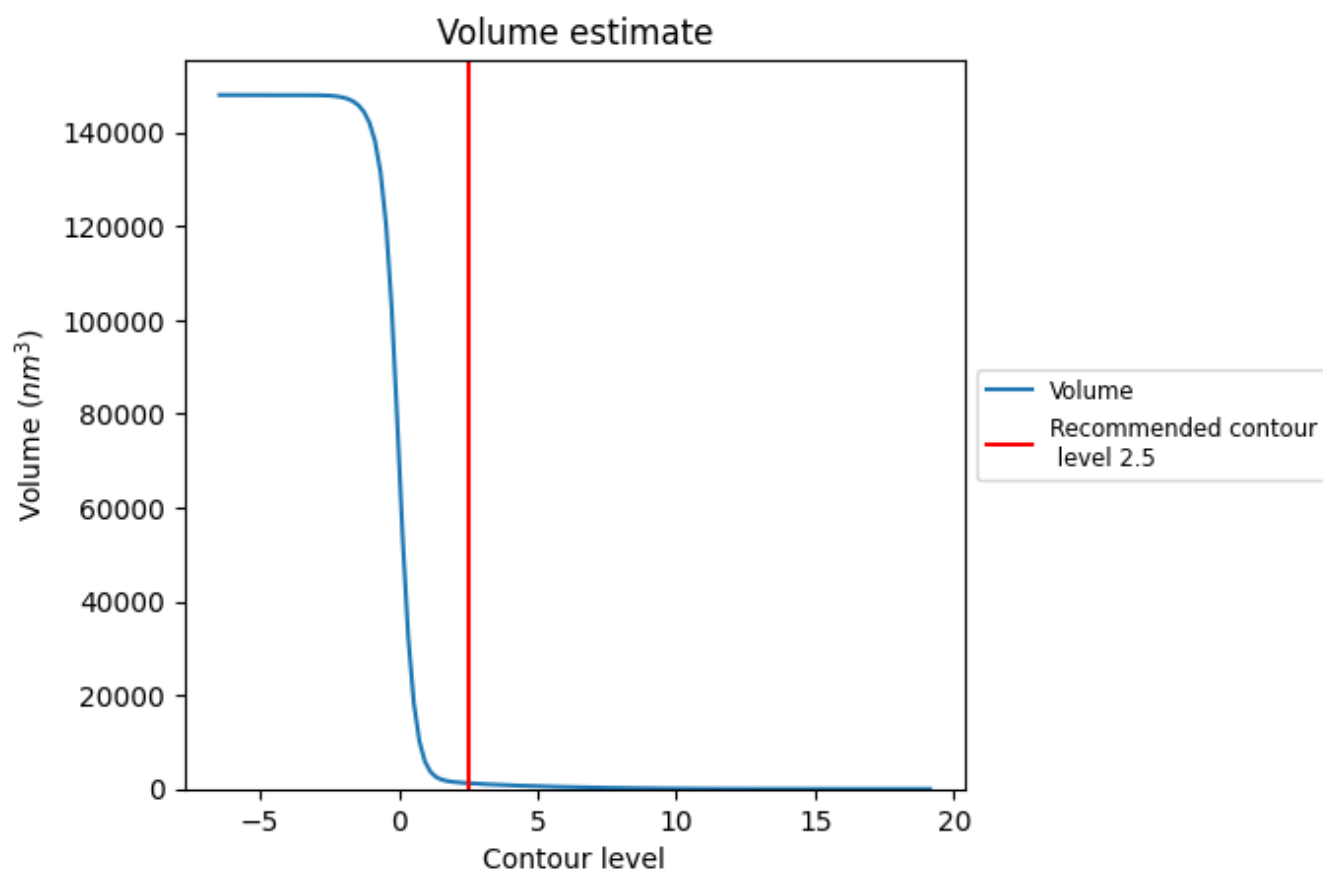
This section contains the results of statistical analysis of the map.

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.

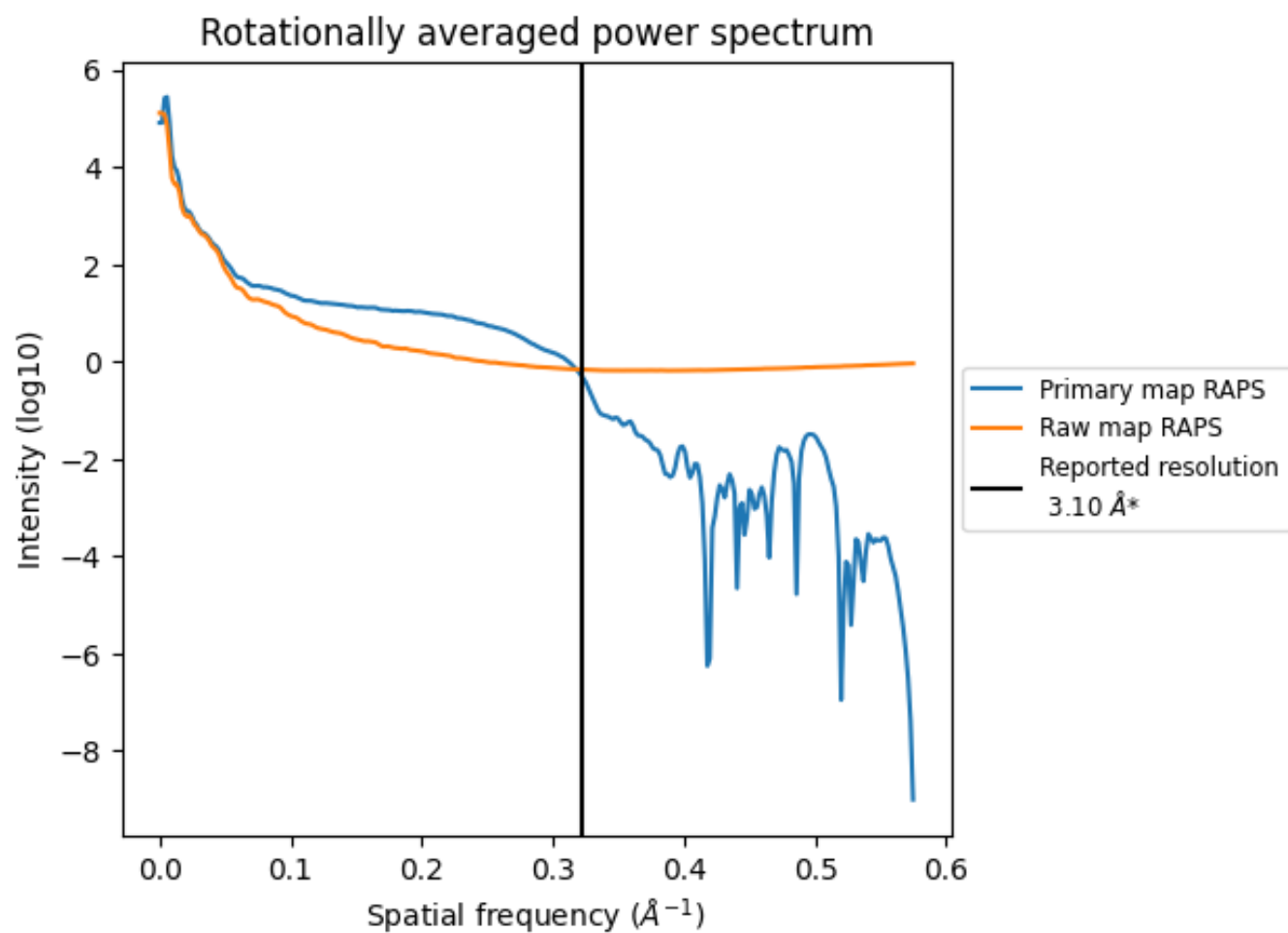
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1232 nm^3 ; this corresponds to an approximate mass of 1112 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 ⓘ

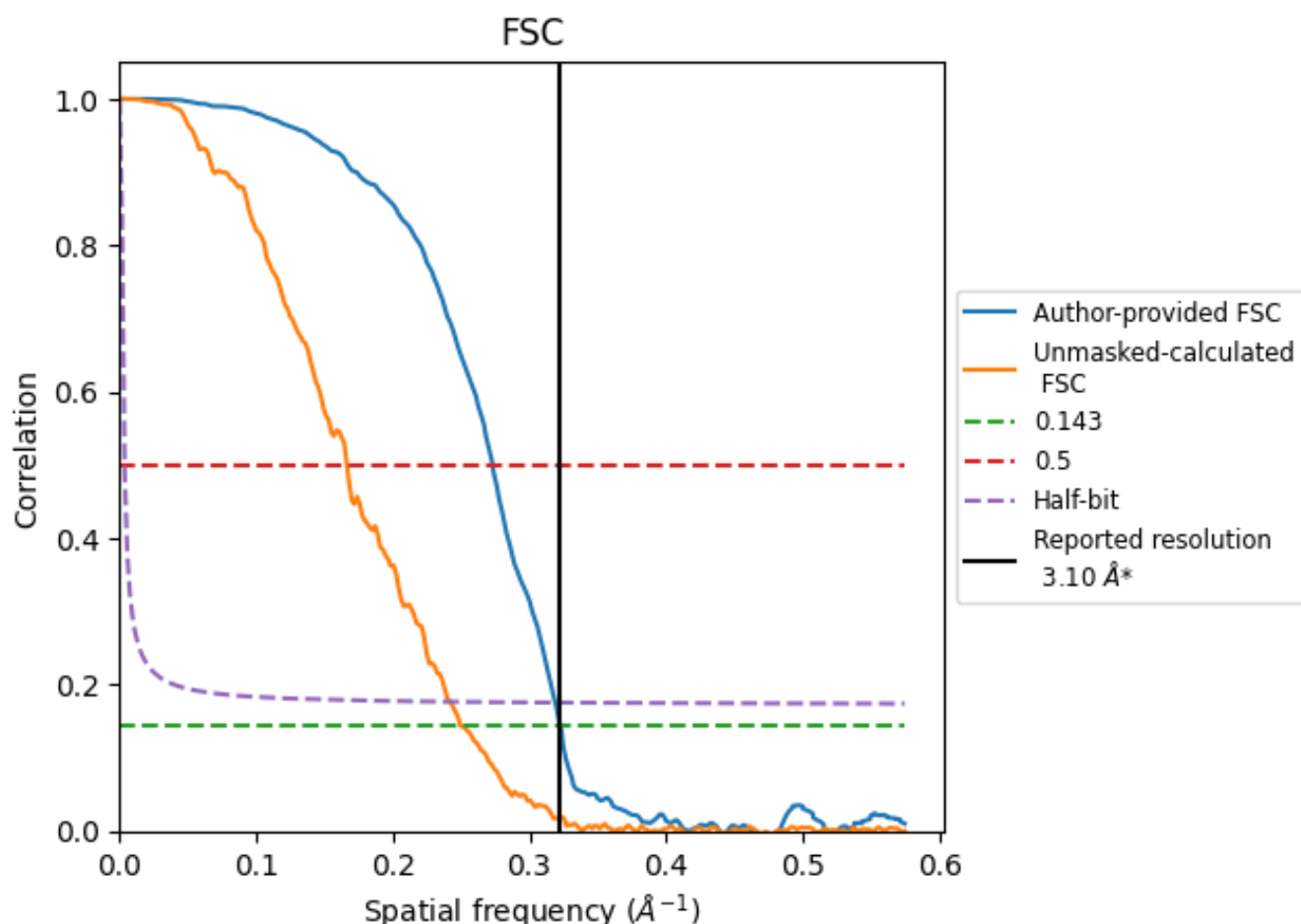


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

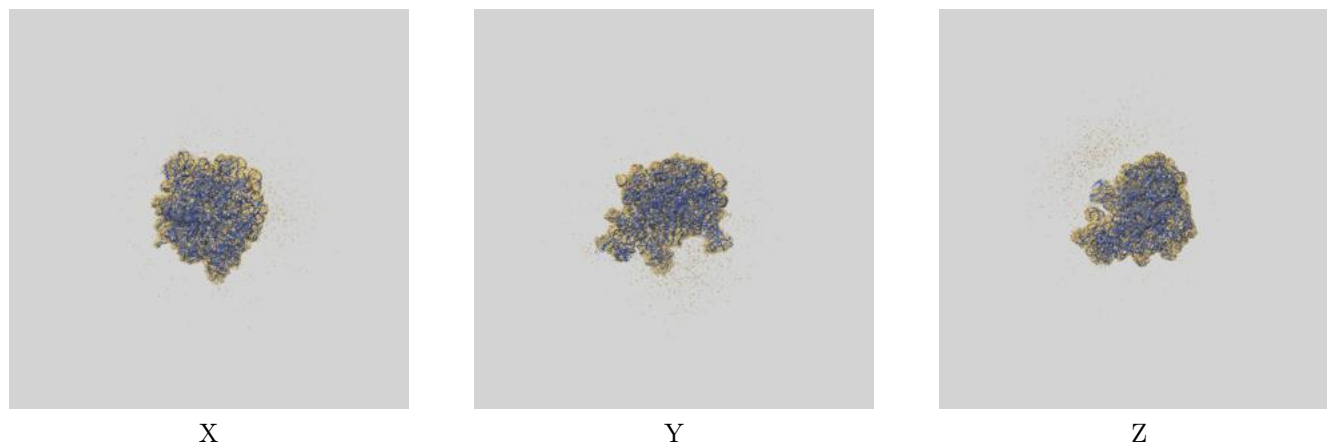
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.66	3.14
Unmasked-calculated*	4.00	6.01	4.13

*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 4.00 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

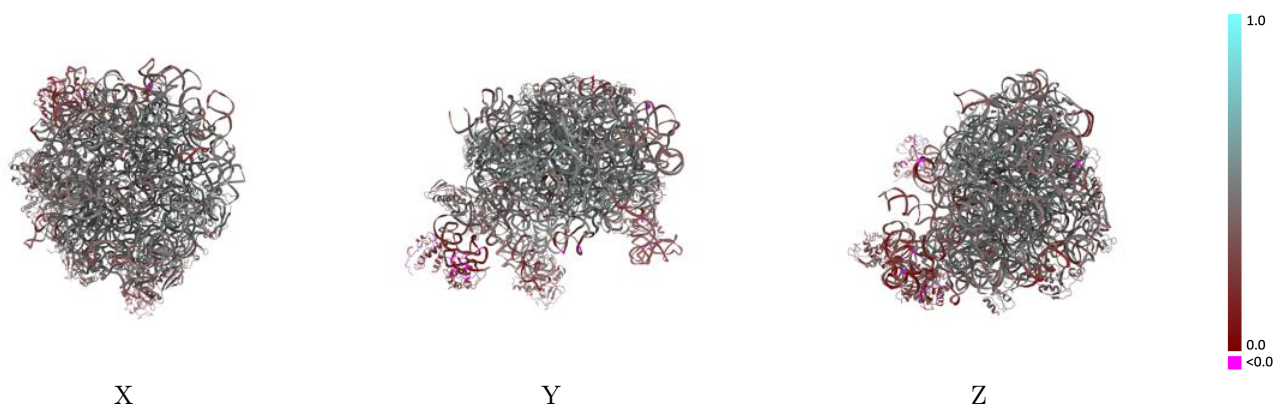
This section contains information regarding the fit between EMDB map EMD-21856 and PDB model 6WNT. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



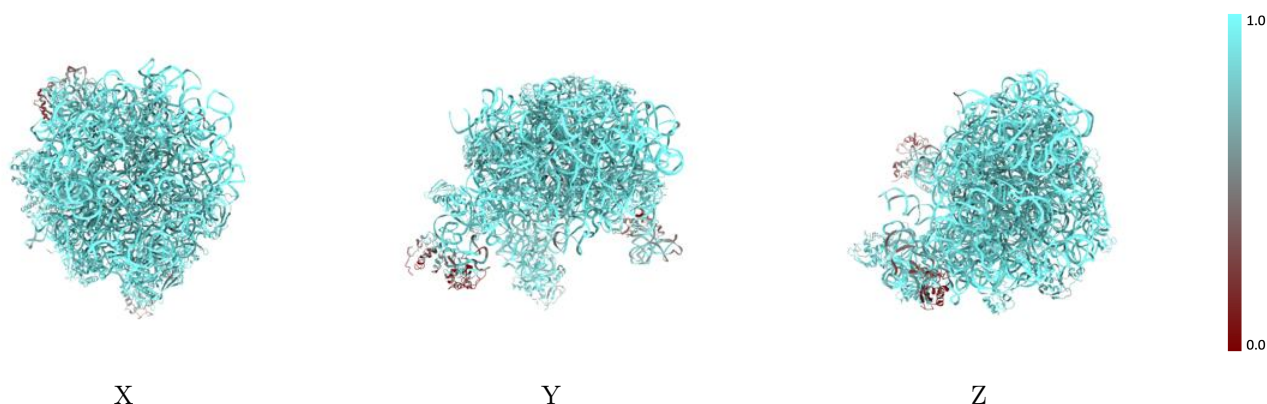
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



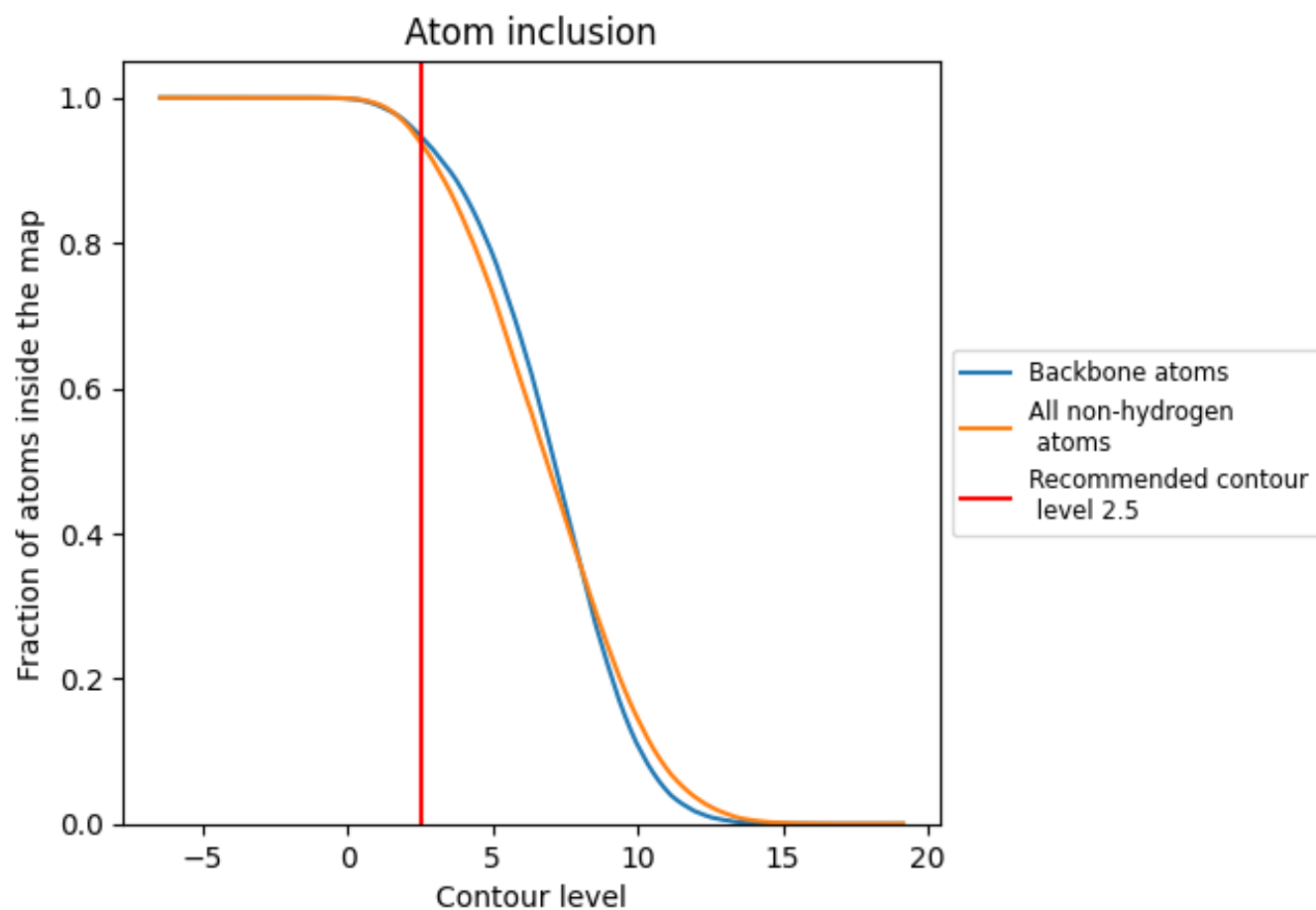
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9391	 0.4250
4	 0.9751	 0.4290
A	 0.7179	 0.3310
B	 0.9368	 0.4790
D	 0.9322	 0.4950
E	 0.9408	 0.4870
F	 0.9075	 0.4750
a	 0.3102	 0.2300
b	 0.9494	 0.4840
c	 0.9239	 0.4780
d	 0.8479	 0.4180
e	 0.8674	 0.3130
f	 0.9174	 0.3960
g	 0.8582	 0.3650
h	 0.4979	 0.2020
i	 0.3242	 0.2000
j	 0.9217	 0.4760
k	 0.9277	 0.4640
l	 0.9300	 0.4590
n	 0.9349	 0.4830
o	 0.9408	 0.3960
p	 0.9064	 0.4570
q	 0.9338	 0.4740
r	 0.9070	 0.4540
s	 0.9042	 0.4740
t	 0.9100	 0.4550
u	 0.9244	 0.4210
v	 0.8372	 0.3310
w	 0.9140	 0.4760
x	 0.9517	 0.4720
y	 0.8972	 0.3890
z	 0.9220	 0.4780

