wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 03:48 AM JST

PDB ID	:	7D6Z
EMDB ID	:	EMD-30598
Title	:	Molecular model of the cryo-EM structure of 70S ribosome in complex with peptide deformylase and trigger factor
Authors	:	Akbar, S.; Bhakta, S.; Sengupta, J.
Deposited on	:	2020-10-02
Resolution	:	3.40 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

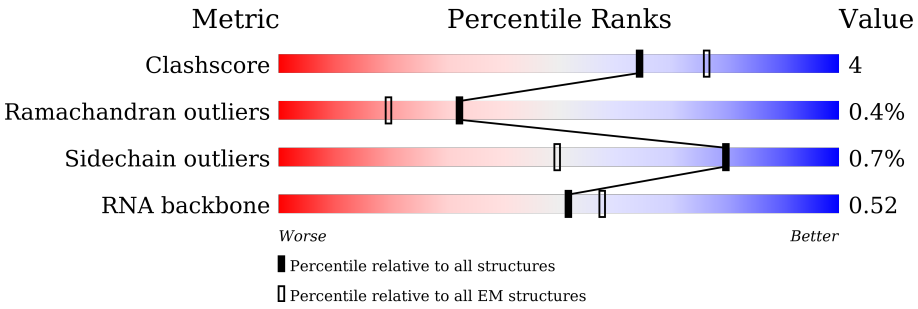
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	0	87	83% 15% ·
2	1	71	54% 17% · 28%
3	2	73	51% 29% 10% 11%
4	3	77	65% 26% 9%
5	4	76	50% 57% 24% 7% 13%
6	6	70	10% 81% 13% 6%
7	A	2903	76% 21% ·

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Mol	Chain	Length	Quality of chain
8	B	118	79% 19%
9	C	273	83% 16%
10	D	209	90% 10%
11	E	201	89% 11%
12	F	179	84% 15%
13	G	177	84% 14%
14	H	149	27% 5% 68%
15	I	142	20% 73% 26%
16	J	142	92% 8%
17	K	123	87% 12%
18	L	144	85% 12%
19	M	136	87% 11%
20	N	127	87% 6% 6%
21	O	117	80% 18%
22	P	115	83% 16%
23	Q	118	91% 8%
24	R	103	88% 12%
25	S	110	92% 8%
26	T	59	88% 10%
27	U	104	82% 15%
28	V	94	94% 6%
29	W	85	82% 6% 12%
30	X	78	85% 14%
31	Y	63	75% 25%
32	Z	100	73% 23%

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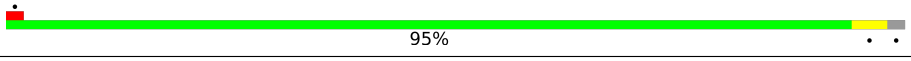
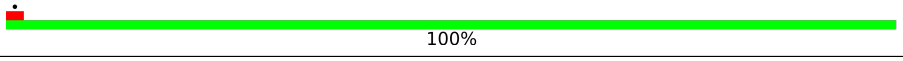
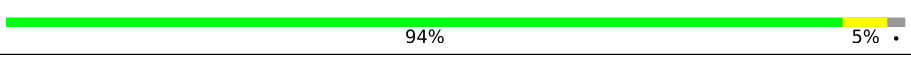
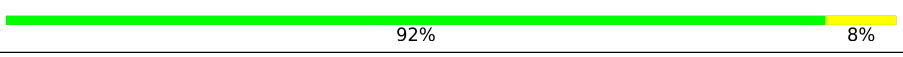
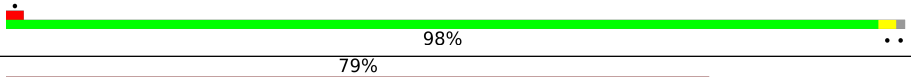
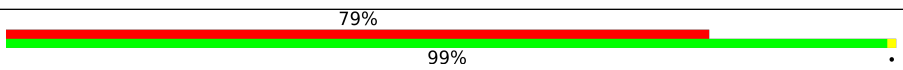
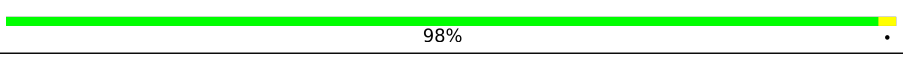
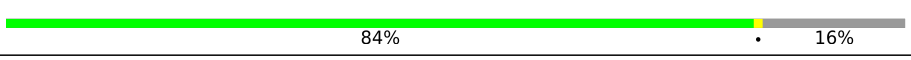
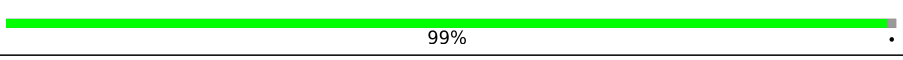
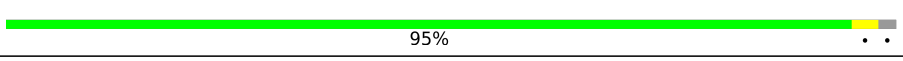
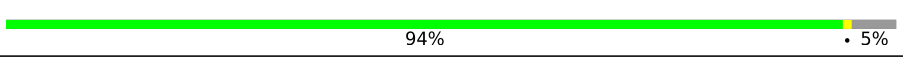
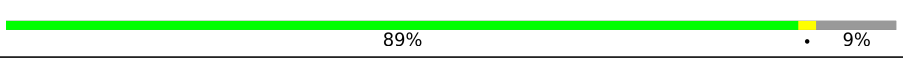
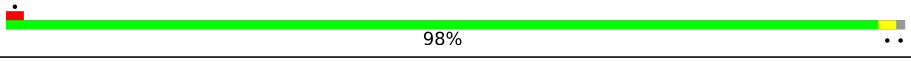
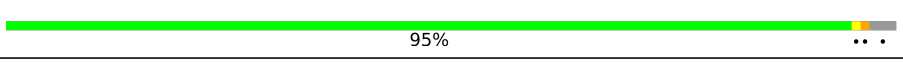
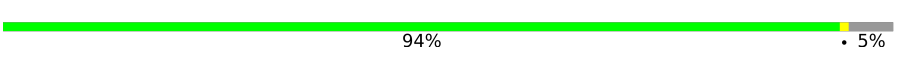
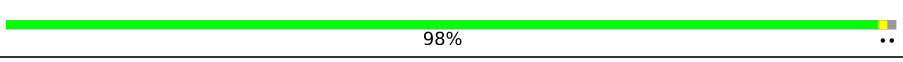
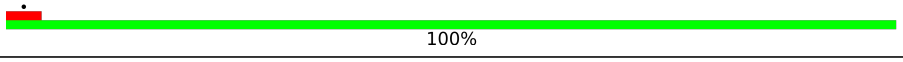
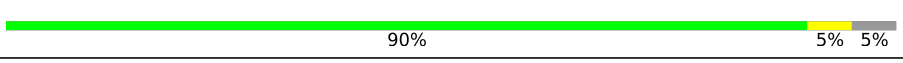
Mol	Chain	Length	Quality of chain
33	a	57	
34	b	55	
35	c	46	
36	d	65	
37	e	38	
38	f	1539	
39	g	169	
40	h	118	
41	i	241	
42	j	233	
43	k	206	
44	l	167	
45	m	135	
46	n	179	
47	o	130	
48	p	130	
49	q	103	
50	r	129	
51	s	124	
52	t	118	
53	u	101	
54	v	89	
55	w	82	
56	x	84	
57	y	75	

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Mol	Chain	Length	Quality of chain
58	z	92	

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 148863 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 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	85	665	411	137	114	3	0	0

- Molecule 2 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	51	425	265	86	73	1	0	0

- Molecule 3 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	65	1392	621	258	449	64	0	0

- Molecule 4 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	3	70	1496	665	267	494	70	0	0

- Molecule 5 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	4	66	1406	629	255	457	65	0	0

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	66	522	323	99	94	6	0	0

- Molecule 7 is a RNA chain called 23S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	2903	Total 62317	C 27801	N 11467	O 20147	P 2902	0	0

- Molecule 8 is a RNA chain called 5S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	118	Total 2529	C 1126	N 464	O 821	P 118	0	0

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	271	Total 2082	C 1288	N 423	O 364	S 7	0	0

- Molecule 10 is a protein called 50S ribosomal protein L3.

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

- Molecule 11 is a protein called 50S ribosomal protein L4.

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

- Molecule 12 is a protein called 50S ribosomal protein L5.

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

- Molecule 13 is a protein called 50S ribosomal protein L6.

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

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

- Molecule 15 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 16 is a protein called 50S ribosomal protein L13.

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

- Molecule 17 is a protein called 50S ribosomal protein L14.

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

- Molecule 18 is a protein called 50S ribosomal protein L15.

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

- Molecule 19 is a protein called 50S ribosomal protein L16.

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

- Molecule 20 is a protein called 50S ribosomal protein L17.

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

- Molecule 21 is a protein called 50S ribosomal protein L18.

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

- Molecule 22 is a protein called 50S ribosomal protein L19.

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

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L21.

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

- Molecule 25 is a protein called 50S ribosomal protein L22.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	U	102	Total 779	C 492	N 146	O 141	0	0

- Molecule 28 is a protein called 50S ribosomal protein L25.

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

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 30 is a protein called 50S ribosomal protein L28.

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

- Molecule 31 is a protein called 50S ribosomal protein L29.

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

- Molecule 32 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	96	Total	C	N	O	S	0	0
			764	484	142	136	2		

- Molecule 33 is a protein called 50S ribosomal protein L32.

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

- Molecule 34 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	b	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 35 is a protein called 50S ribosomal protein L34.

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

- Molecule 36 is a protein called 50S ribosomal protein L35.

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

- Molecule 37 is a protein called 50S ribosomal protein L36.

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

- Molecule 38 is a RNA chain called 16S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 39 is a protein called Peptide deformylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	168	Total	C	N	O	S	0	0
			1346	844	241	255	6		

- Molecule 40 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	118	Total	C	N	O	S	0	0
			919	583	157	176	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	0	HIS	-	expression tag	UNP P0A850

- Molecule 41 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 42 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 43 is a protein called 30S ribosomal protein S4.

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

- Molecule 44 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 45 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 46 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 47 is a protein called 30S ribosomal protein S8.

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

- Molecule 48 is a protein called 30S ribosomal protein S9.

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

- Molecule 49 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 50 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 51 is a protein called 30S ribosomal protein S12.

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

- Molecule 52 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 53 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 54 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

- Molecule 55 is a protein called 30S ribosomal protein S16.

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

- Molecule 56 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	80	Total 648	C 411	N 121	O 113	S 3	0	0

- Molecule 57 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	y	55	Total 455	C 288	N 86	O 81	0	0

- Molecule 58 is a protein called 30S ribosomal protein S19.

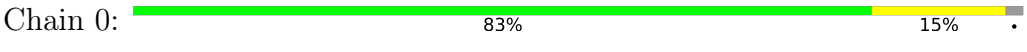
Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	79	Total 637	C 408	N 120	O 107	S 2	0	0

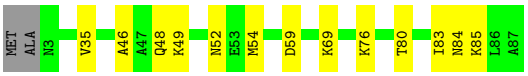
3 Residue-property plots

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: 30S ribosomal protein S20

Chain 0:



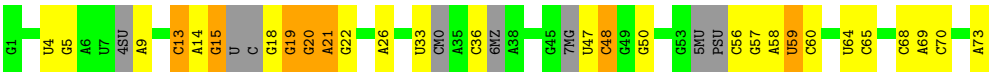


- Molecule 2: 30S ribosomal protein S21

Chain 1:

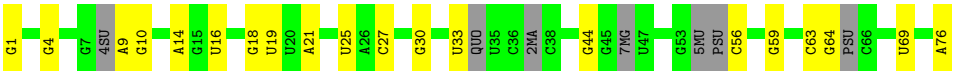
- Molecule 3: E-site tRNA

Chain 2:



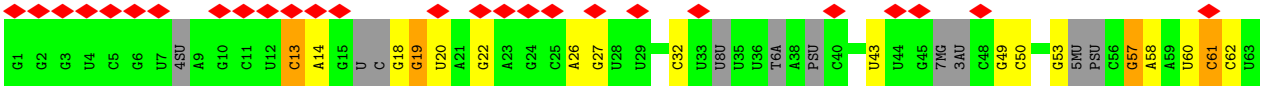
- Molecule 4: P-site tRNA

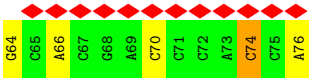
Chain 3:



- Molecule 5: A-site tRNA

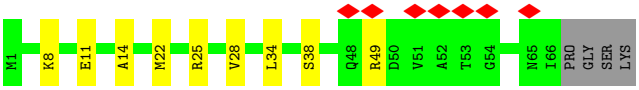
Chain 4:





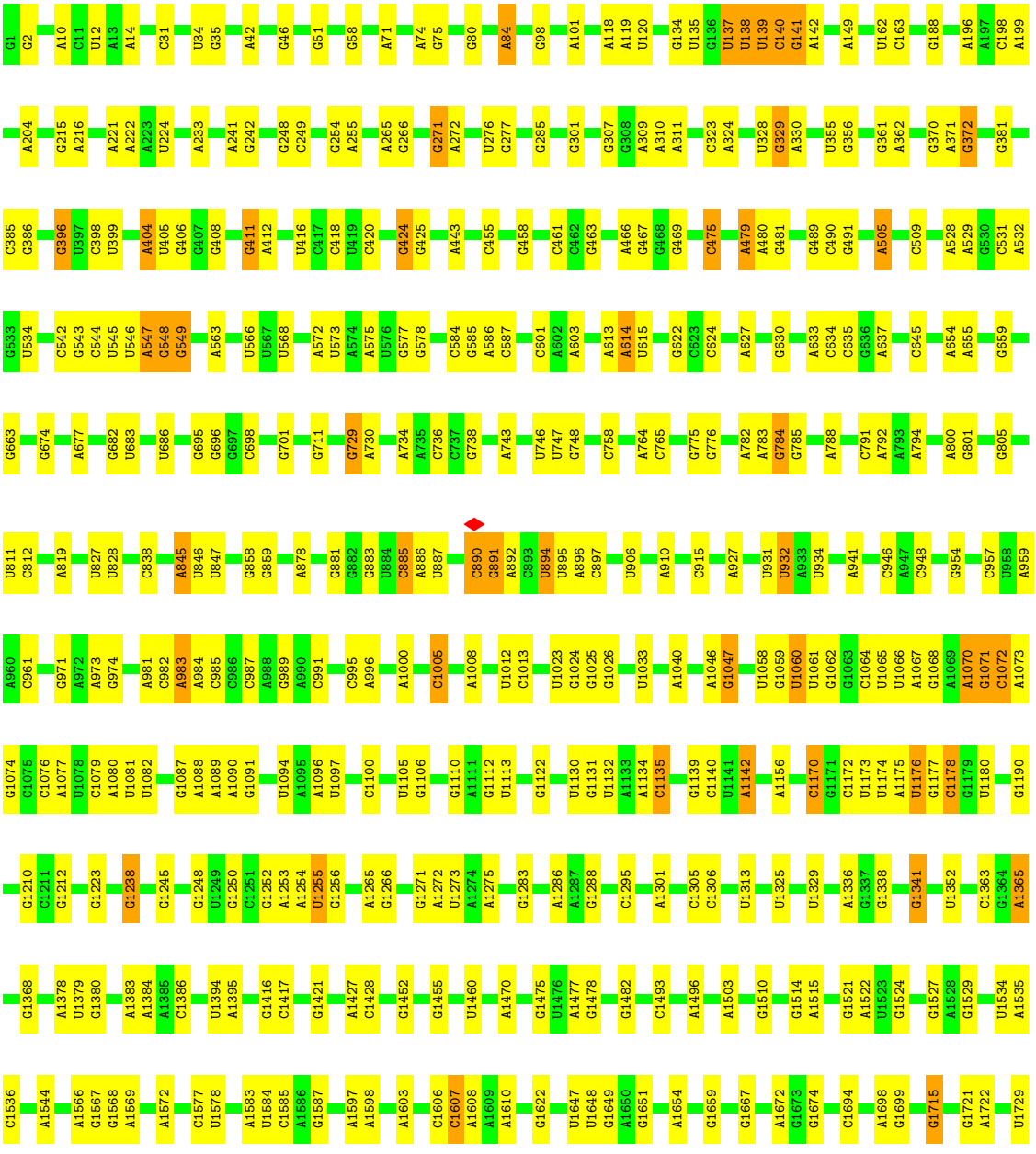
• Molecule 6: 50S ribosomal protein L31

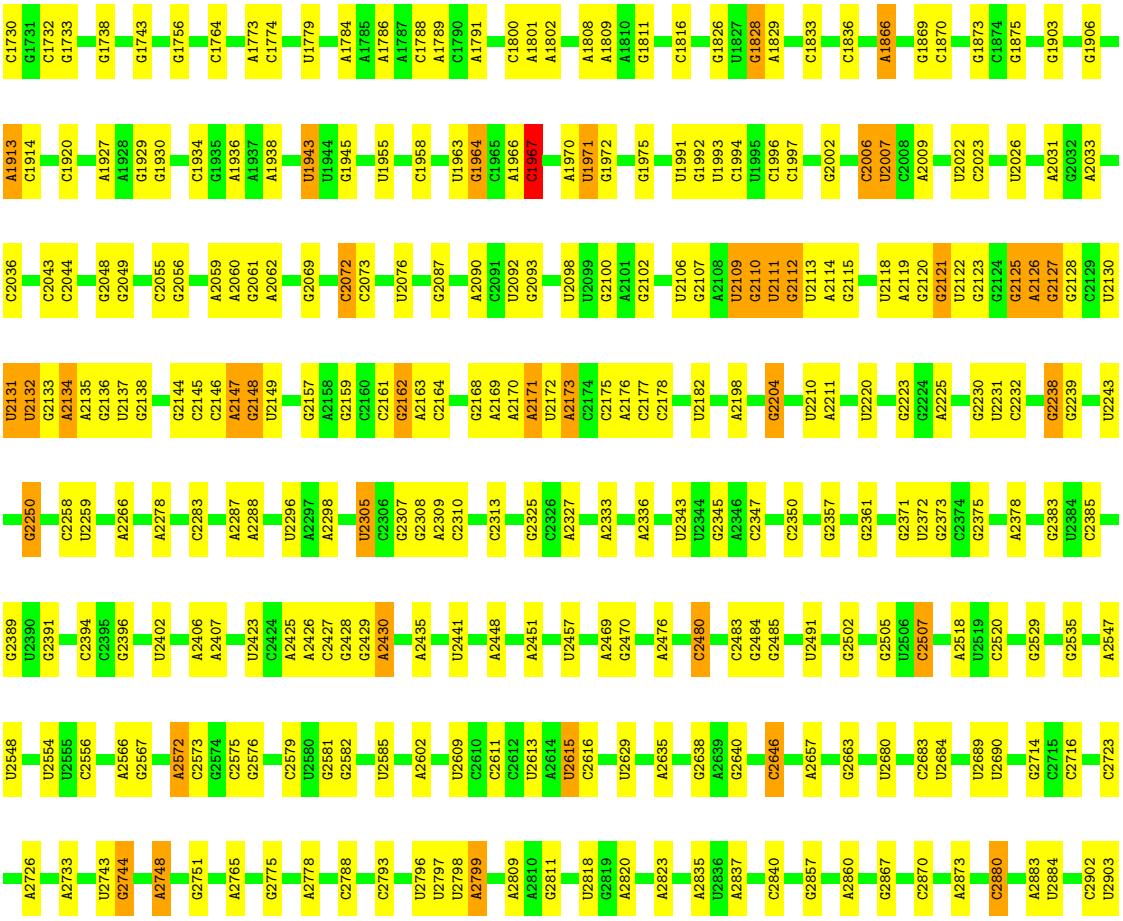
Chain 6:



• Molecule 7: 23S ribosomal rRNA

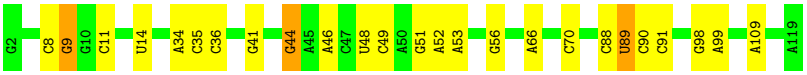
Chain A:





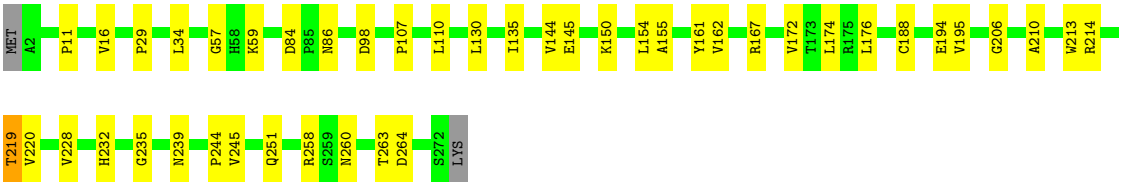
• Molecule 8: 5S ribosomal rRNA

Chain B:



• Molecule 9: 50S ribosomal protein L2

Chain C:

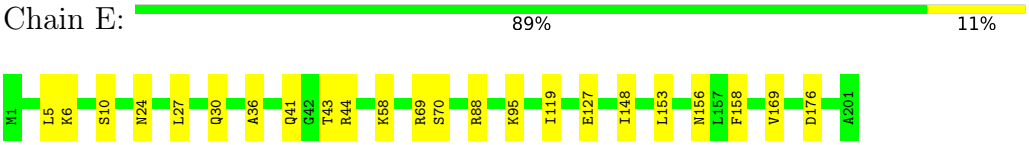


• Molecule 10: 50S ribosomal protein L3

Chain D:

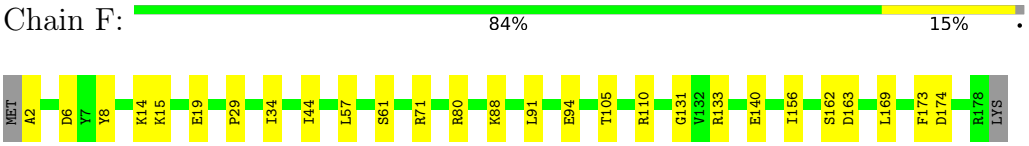
• Molecule 11: 50S ribosomal protein L4

Chain E:



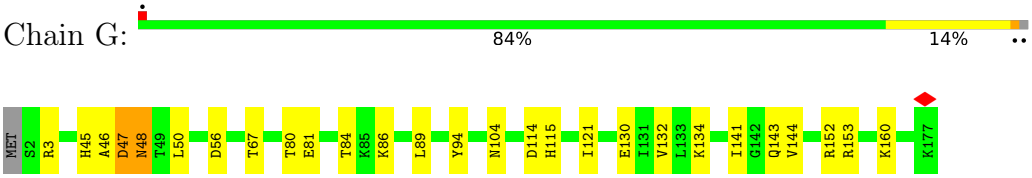
• Molecule 12: 50S ribosomal protein L5

Chain F:



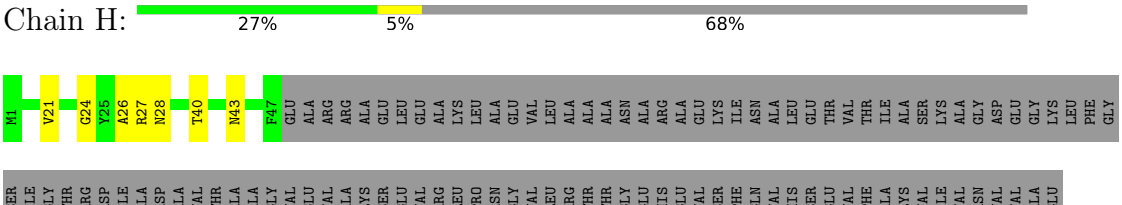
• Molecule 13: 50S ribosomal protein L6

Chain G:



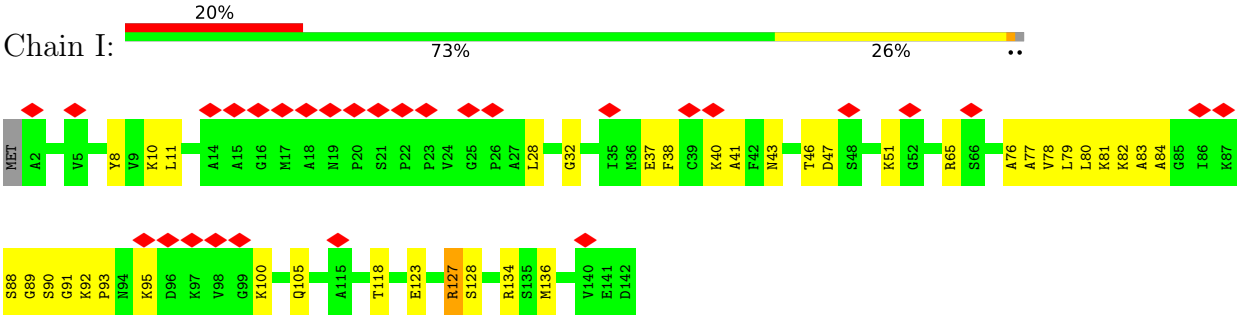
• Molecule 14: 50S ribosomal protein L9

Chain H:



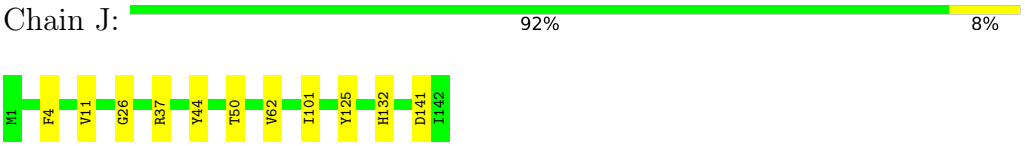
• Molecule 15: 50S ribosomal protein L11

Chain I:



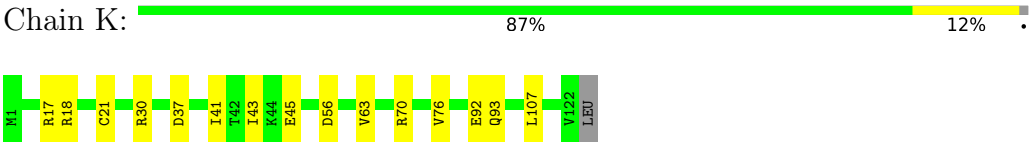
• Molecule 16: 50S ribosomal protein L13

Chain J:



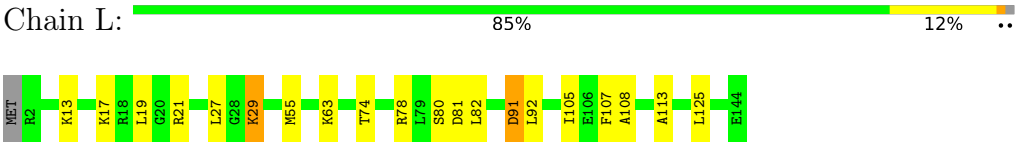
• Molecule 17: 50S ribosomal protein L14

Chain K:



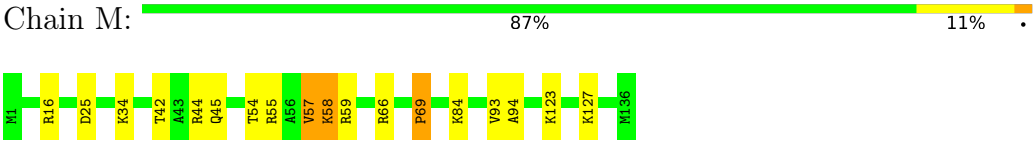
• Molecule 18: 50S ribosomal protein L15

Chain L:



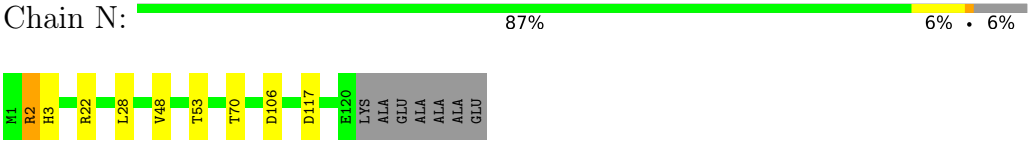
• Molecule 19: 50S ribosomal protein L16

Chain M:



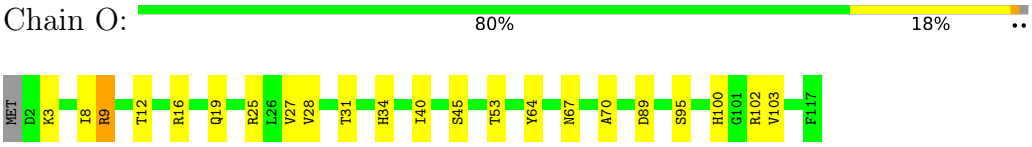
• Molecule 20: 50S ribosomal protein L17

Chain N:



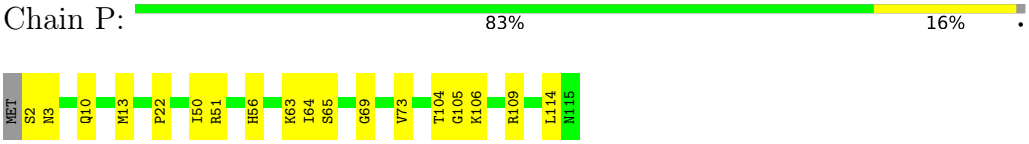
• Molecule 21: 50S ribosomal protein L18

Chain O:



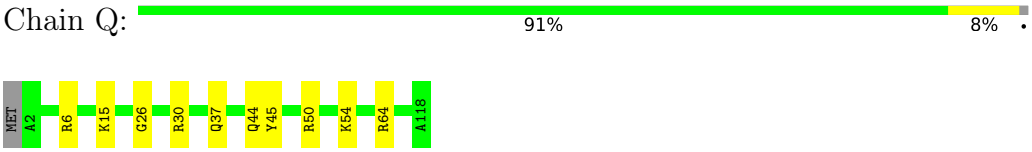
• Molecule 22: 50S ribosomal protein L19

Chain P:



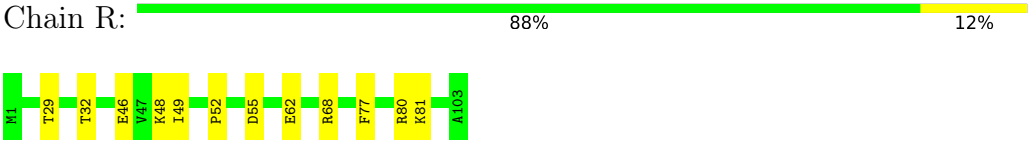
• Molecule 23: 50S ribosomal protein L20

Chain Q:



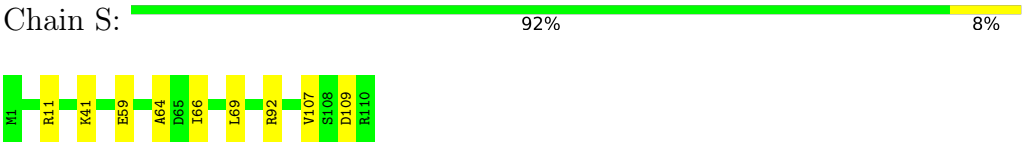
• Molecule 24: 50S ribosomal protein L21

Chain R:



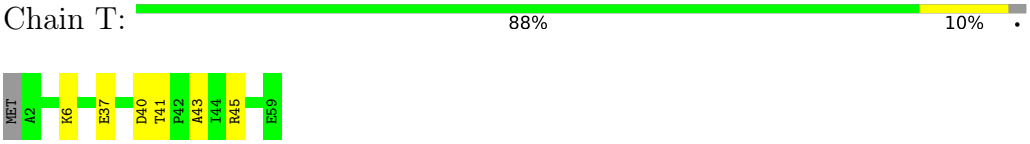
• Molecule 25: 50S ribosomal protein L22

Chain S:



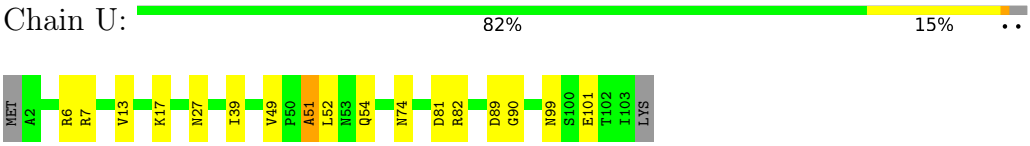
• Molecule 26: 50S ribosomal protein L30

Chain T:



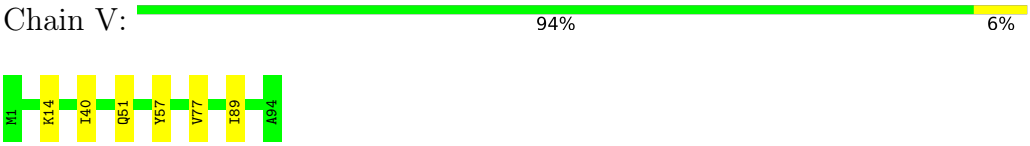
• Molecule 27: 50S ribosomal protein L24

Chain U:



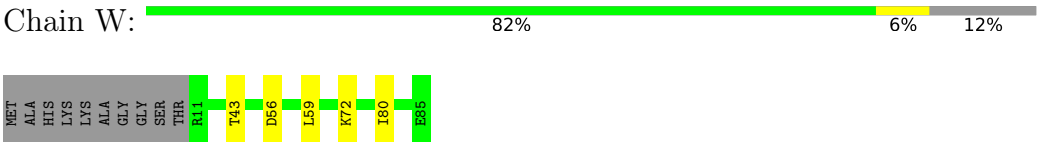
• Molecule 28: 50S ribosomal protein L25

Chain V:



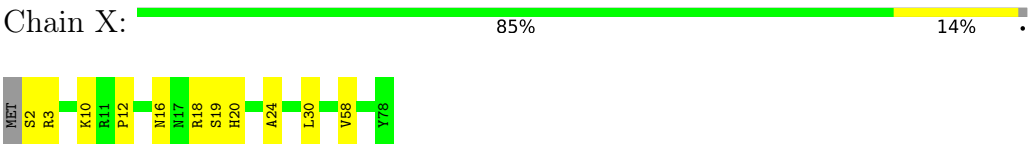
• Molecule 29: 50S ribosomal protein L27

Chain W:



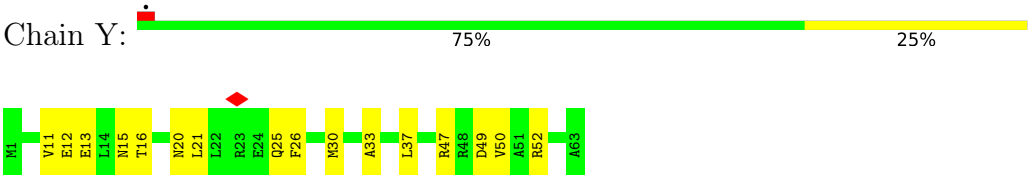
• Molecule 30: 50S ribosomal protein L28

Chain X:



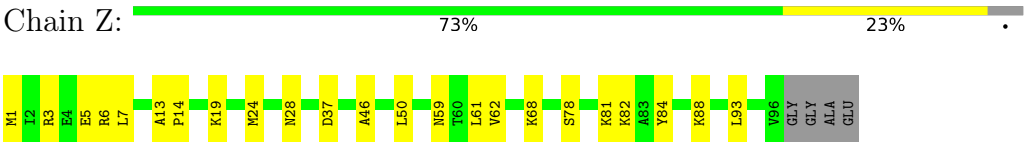
• Molecule 31: 50S ribosomal protein L29

Chain Y:



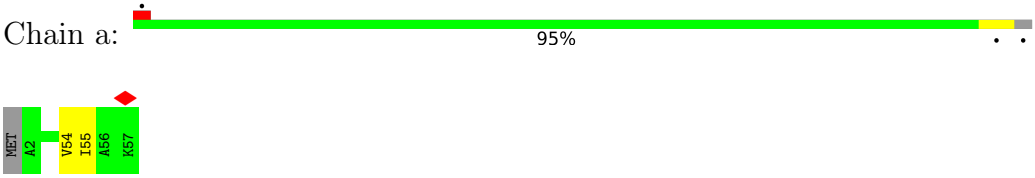
• Molecule 32: 50S ribosomal protein L23

Chain Z:



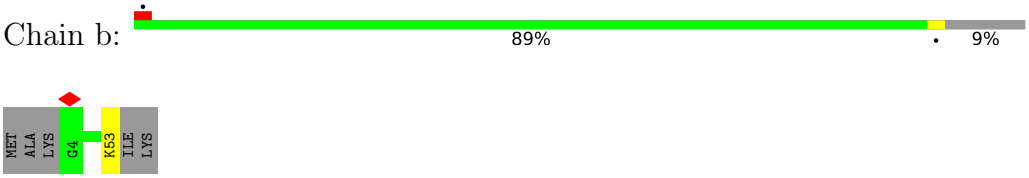
• Molecule 33: 50S ribosomal protein L32

Chain a:



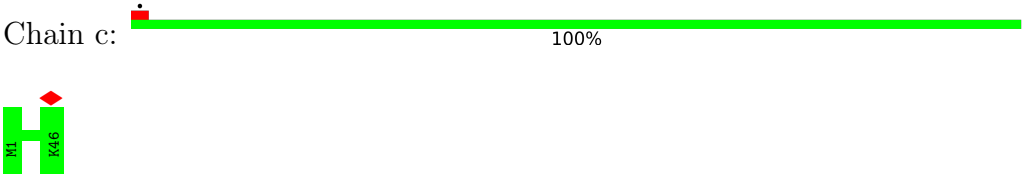
• Molecule 34: 50S ribosomal protein L33

Chain b:



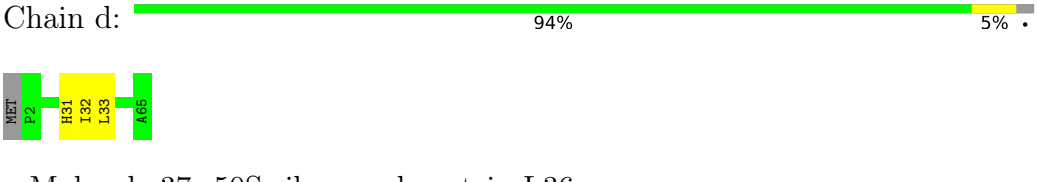
• Molecule 35: 50S ribosomal protein L34

Chain c:



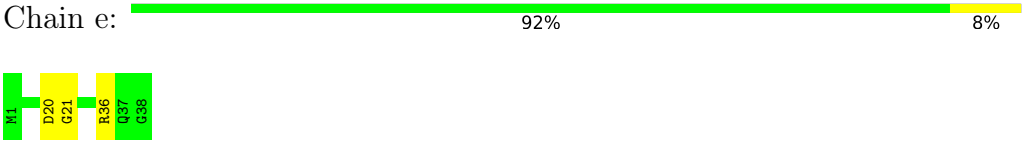
• Molecule 36: 50S ribosomal protein L35

Chain d:



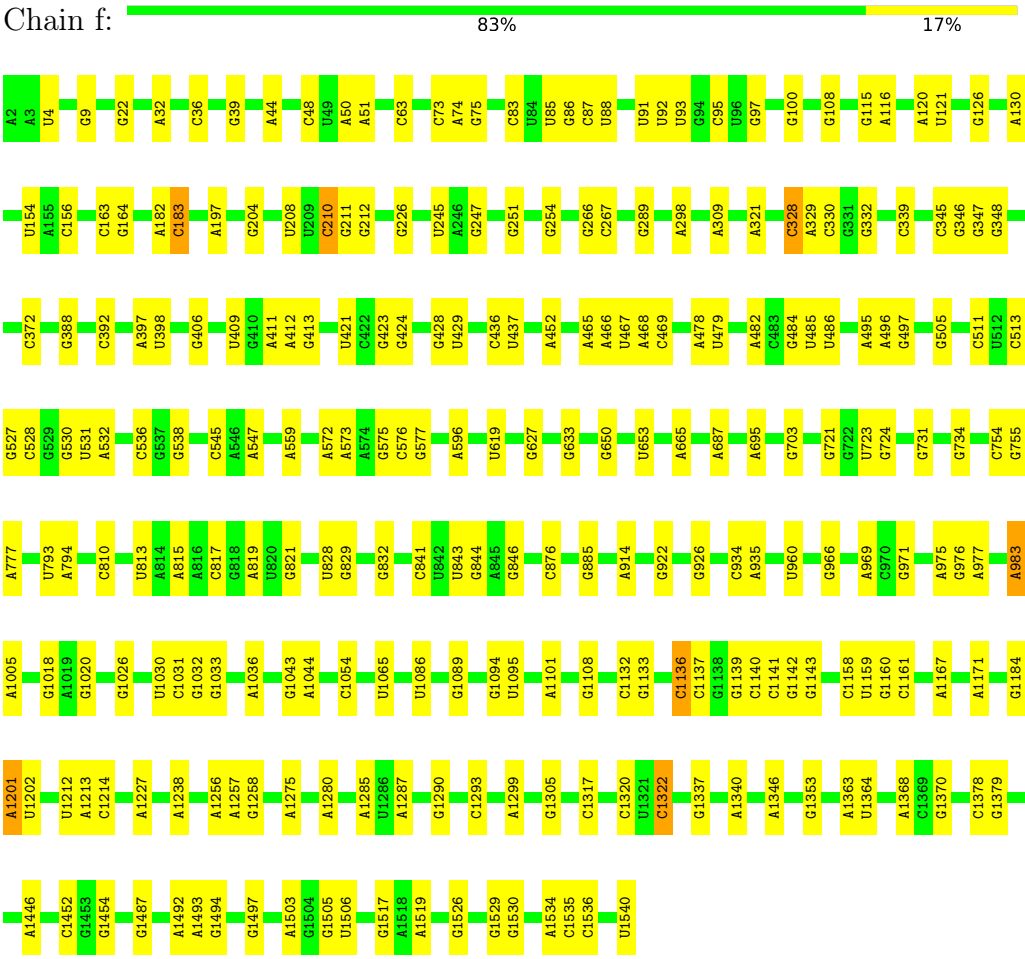
• Molecule 37: 50S ribosomal protein L36

Chain e:



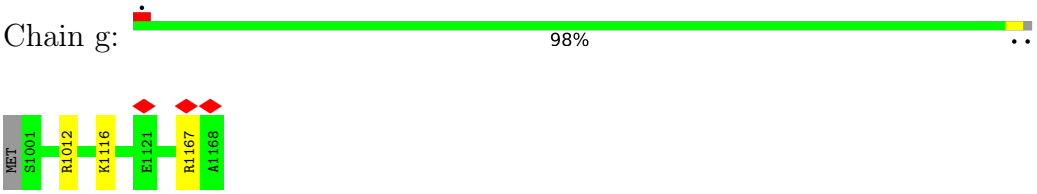
• Molecule 38: 16S ribosomal rRNA

Chain f:



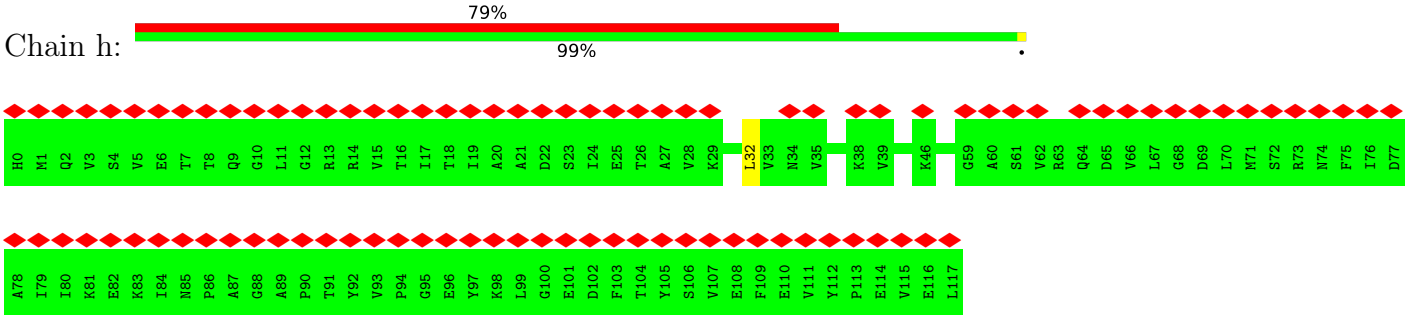
• Molecule 39: Peptide deformylase

Chain g:



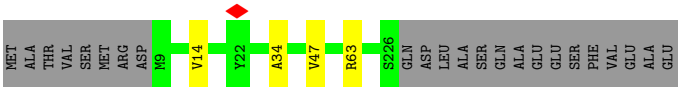
• Molecule 40: Trigger factor

Chain h:



• Molecule 41: 30S ribosomal protein S2

Chain i:

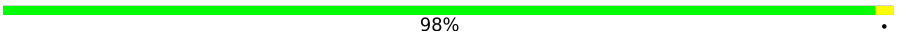


• Molecule 42: 30S ribosomal protein S3

Chain j:

• Molecule 43: 30S ribosomal protein S4

Chain k:



• Molecule 44: 30S ribosomal protein S5

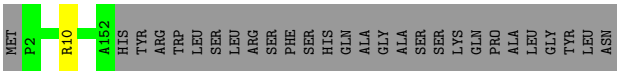
Chain l:

• Molecule 45: 30S ribosomal protein S6, fully modified isoform

Chain m:

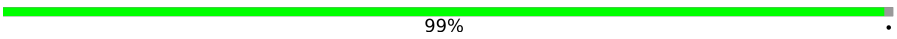
• Molecule 46: 30S ribosomal protein S7

Chain n:



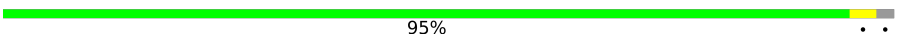
• Molecule 47: 30S ribosomal protein S8

Chain o:



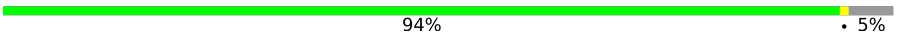
• Molecule 48: 30S ribosomal protein S9

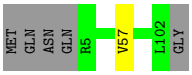
Chain p:



• Molecule 49: 30S ribosomal protein S10

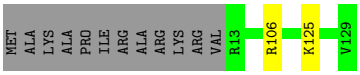
Chain q:





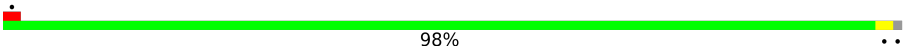
• Molecule 50: 30S ribosomal protein S11

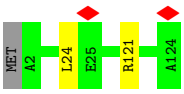
Chain r:



• Molecule 51: 30S ribosomal protein S12

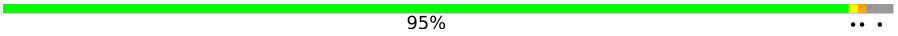
Chain s:





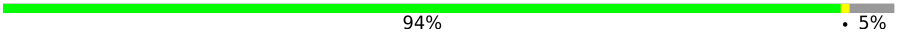
• Molecule 52: 30S ribosomal protein S13

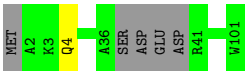
Chain t:



• Molecule 53: 30S ribosomal protein S14

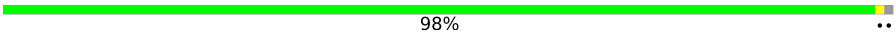
Chain u:

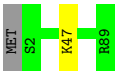




• Molecule 54: 30S ribosomal protein S15

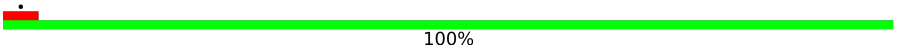
Chain v:

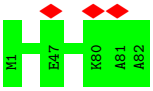




• Molecule 55: 30S ribosomal protein S16

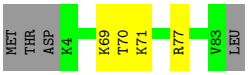
Chain w:





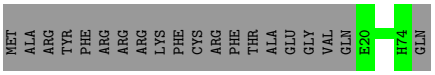
• Molecule 56: 30S ribosomal protein S17

Chain x:



• Molecule 57: 30S ribosomal protein S18

Chain y:



• Molecule 58: 30S ribosomal protein S19

Chain z:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	194157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32.57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	25.576	Depositor
Minimum map value	-14.991	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	441.6, 441.6, 441.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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	0	0.27	0/671	0.50	0/888
2	1	0.35	0/430	0.74	2/570 (0.4%)
3	2	0.28	0/1551	0.89	1/2404 (0.0%)
4	3	0.49	1/1664 (0.1%)	0.89	0/2577
5	4	0.26	0/1565	0.92	1/2421 (0.0%)
6	6	0.28	0/531	0.51	0/709
7	A	0.87	2/69796 (0.0%)	0.95	77/108888 (0.1%)
8	B	0.66	0/2828	0.89	1/4410 (0.0%)
9	C	0.50	0/2121	0.61	1/2852 (0.0%)
10	D	0.48	0/1586	0.57	0/2134
11	E	0.44	0/1571	0.53	0/2113
12	F	0.32	0/1434	0.52	0/1926
13	G	0.35	0/1343	0.52	0/1816
14	H	0.36	0/364	0.69	0/490
15	I	0.28	0/1046	0.60	1/1410 (0.1%)
16	J	0.46	0/1152	0.51	0/1551
17	K	0.46	0/947	0.63	0/1268
18	L	0.44	0/1054	0.65	1/1403 (0.1%)
19	M	0.43	0/1093	0.57	0/1460
20	N	0.44	0/973	0.62	0/1301
21	O	0.37	0/902	0.50	0/1209
22	P	0.45	0/929	0.56	1/1242 (0.1%)
23	Q	0.53	0/960	0.52	0/1278
24	R	0.46	0/829	0.57	0/1107
25	S	0.42	0/864	0.52	0/1156
26	T	0.40	0/453	0.58	0/605
27	U	0.42	0/787	0.57	0/1051
28	V	0.38	0/766	0.50	0/1025
29	W	0.45	0/576	0.51	0/762
30	X	0.45	0/635	0.49	0/848
31	Y	0.36	0/510	0.51	0/677
32	Z	0.39	0/771	0.63	0/1031
33	a	0.43	0/450	0.62	0/599
34	b	0.35	0/416	0.53	0/554

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	c	0.46	0/380	0.56	0/498
36	d	0.44	0/513	0.66	0/676
37	e	0.45	0/303	0.59	0/397
38	f	0.59	0/36966	0.89	28/57666 (0.0%)
39	g	0.28	0/1361	0.58	0/1830
40	h	0.28	0/933	0.57	1/1261 (0.1%)
41	i	0.32	0/1735	0.56	0/2338
42	j	0.32	0/1651	0.52	0/2225
43	k	0.32	0/1665	0.58	0/2227
44	l	0.39	0/1118	0.63	0/1504
45	m	0.34	0/835	0.65	1/1128 (0.1%)
46	n	0.29	0/1195	0.48	0/1602
47	o	0.36	0/989	0.50	0/1326
48	p	0.31	0/1034	0.57	0/1375
49	q	0.31	0/796	0.58	0/1077
50	r	0.35	0/893	0.55	0/1205
51	s	0.36	0/969	0.60	0/1300
52	t	0.30	0/892	0.56	0/1193
53	u	0.30	0/785	0.52	0/1043
54	v	0.32	0/718	0.53	0/959
55	w	0.29	0/659	0.56	0/884
56	x	0.32	0/657	0.67	0/881
57	y	0.34	0/462	0.51	0/621
58	z	0.30	0/652	0.52	0/877
All	All	0.68	3/161729 (0.0%)	0.85	116/241828 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	D	0	1
12	F	0	1
13	G	0	2
17	K	0	1
18	L	0	1
19	M	0	2
20	N	0	1
27	U	0	2
33	a	0	1
36	d	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	e	0	1
41	i	0	1
43	k	0	1
44	l	0	2
45	m	0	2
48	p	0	1
51	s	0	1
52	t	0	1
56	x	0	2
All	All	0	25

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	1	G	OP3-P	-10.68	1.48	1.61
7	A	1142	A	N9-C4	-5.69	1.34	1.37
7	A	528	A	N9-C4	-5.29	1.34	1.37

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	f	328	C	N1-C2-O2	9.60	124.66	118.90
45	m	54	LEU	CA-CB-CG	9.20	136.46	115.30
38	f	328	C	C2-N1-C1'	8.62	128.28	118.80
7	A	12	U	N3-C2-O2	-8.44	116.30	122.20
38	f	328	C	N3-C2-O2	-8.14	116.20	121.90

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	D	151	THR	Peptide
12	F	174	ASP	Peptide
13	G	46	ALA	Peptide
13	G	47	ASP	Peptide
17	K	92	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	665	0	714	9	0
2	1	425	0	449	7	0
3	2	1392	0	714	16	0
4	3	1496	0	764	7	0
5	4	1406	0	722	6	0
6	6	522	0	522	6	0
7	A	62317	0	31345	179	0
8	B	2529	0	1281	11	0
9	C	2082	0	2154	26	0
10	D	1565	0	1616	14	0
11	E	1552	0	1619	15	0
12	F	1410	0	1444	18	0
13	G	1323	0	1371	17	0
14	H	359	0	381	5	0
15	I	1032	0	1085	25	0
16	J	1129	0	1162	7	0
17	K	938	0	1012	9	0
18	L	1045	0	1117	17	0
19	M	1074	0	1157	13	0
20	N	960	0	1000	5	0
21	O	892	0	923	17	0
22	P	917	0	962	10	0
23	Q	947	0	1019	8	0
24	R	816	0	839	9	0
25	S	857	0	922	5	0
26	T	449	0	488	4	0
27	U	779	0	831	8	0
28	V	753	0	780	4	0
29	W	569	0	581	4	0
30	X	625	0	652	8	0
31	Y	509	0	543	18	0
32	Z	764	0	829	26	0
33	a	444	0	458	0	0
34	b	409	0	440	0	0
35	c	377	0	418	0	0
36	d	504	0	572	0	0
37	e	302	0	343	0	0
38	f	33015	0	16617	0	0
39	g	1346	0	1391	0	0
40	h	919	0	938	0	0
41	i	1704	0	1732	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	j	1624	0	1696	0	0
43	k	1643	0	1707	0	0
44	l	1105	0	1148	0	0
45	m	817	0	808	0	0
46	n	1181	0	1238	0	0
47	o	979	0	1031	0	0
48	p	1022	0	1070	0	0
49	q	786	0	828	0	0
50	r	877	0	887	0	0
51	s	955	0	1016	0	0
52	t	883	0	941	0	0
53	u	774	0	824	0	0
54	v	710	0	728	0	0
55	w	649	0	666	0	0
56	x	648	0	691	0	0
57	y	455	0	478	0	0
58	z	637	0	665	0	0
All	All	148863	0	100329	435	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 435 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Y:21:LEU:CD1	32:Z:5:GLU:OE2	1.82	1.28
31:Y:21:LEU:HD13	32:Z:5:GLU:OE2	1.33	1.25
31:Y:21:LEU:HD11	32:Z:5:GLU:OE2	1.70	0.91
31:Y:33:ALA:CB	32:Z:13:ALA:HB1	2.03	0.88
31:Y:33:ALA:HB2	32:Z:13:ALA:CB	2.18	0.74

There are no symmetry-related clashes.

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	0	83/87 (95%)	77 (93%)	5 (6%)	1 (1%)	11 35
2	1	49/71 (69%)	34 (69%)	15 (31%)	0	100 100
6	6	64/70 (91%)	55 (86%)	9 (14%)	0	100 100
9	C	269/273 (98%)	241 (90%)	28 (10%)	0	100 100
10	D	207/209 (99%)	194 (94%)	12 (6%)	1 (0%)	25 54
11	E	199/201 (99%)	191 (96%)	8 (4%)	0	100 100
12	F	175/179 (98%)	159 (91%)	16 (9%)	0	100 100
13	G	174/177 (98%)	160 (92%)	12 (7%)	2 (1%)	12 37
14	H	45/149 (30%)	35 (78%)	10 (22%)	0	100 100
15	I	139/142 (98%)	112 (81%)	27 (19%)	0	100 100
16	J	140/142 (99%)	133 (95%)	7 (5%)	0	100 100
17	K	120/123 (98%)	101 (84%)	18 (15%)	1 (1%)	16 44
18	L	141/144 (98%)	122 (86%)	18 (13%)	1 (1%)	19 47
19	M	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	5 24
20	N	118/127 (93%)	103 (87%)	14 (12%)	1 (1%)	16 44
21	O	114/117 (97%)	106 (93%)	8 (7%)	0	100 100
22	P	112/115 (97%)	99 (88%)	13 (12%)	0	100 100
23	Q	115/118 (98%)	114 (99%)	1 (1%)	0	100 100
24	R	101/103 (98%)	92 (91%)	9 (9%)	0	100 100
25	S	108/110 (98%)	103 (95%)	5 (5%)	0	100 100
26	T	56/59 (95%)	53 (95%)	3 (5%)	0	100 100
27	U	100/104 (96%)	85 (85%)	12 (12%)	3 (3%)	3 19
28	V	92/94 (98%)	87 (95%)	5 (5%)	0	100 100
29	W	73/85 (86%)	71 (97%)	2 (3%)	0	100 100
30	X	75/78 (96%)	71 (95%)	4 (5%)	0	100 100
31	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100 100
32	Z	94/100 (94%)	82 (87%)	12 (13%)	0	100 100
33	a	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	6 26
34	b	48/55 (87%)	47 (98%)	1 (2%)	0	100 100
35	c	44/46 (96%)	43 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
36	d	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3 18
37	e	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4 20
39	g	166/169 (98%)	158 (95%)	8 (5%)	0	100 100
40	h	116/118 (98%)	105 (90%)	11 (10%)	0	100 100
41	i	216/241 (90%)	185 (86%)	31 (14%)	0	100 100
42	j	204/233 (88%)	181 (89%)	23 (11%)	0	100 100
43	k	203/206 (98%)	167 (82%)	36 (18%)	0	100 100
44	l	148/167 (89%)	119 (80%)	29 (20%)	0	100 100
45	m	98/135 (73%)	85 (87%)	13 (13%)	0	100 100
46	n	149/179 (83%)	141 (95%)	8 (5%)	0	100 100
47	o	127/130 (98%)	122 (96%)	5 (4%)	0	100 100
48	p	125/130 (96%)	106 (85%)	18 (14%)	1 (1%)	16 44
49	q	96/103 (93%)	82 (85%)	13 (14%)	1 (1%)	13 39
50	r	115/129 (89%)	99 (86%)	16 (14%)	0	100 100
51	s	121/124 (98%)	100 (83%)	21 (17%)	0	100 100
52	t	112/118 (95%)	103 (92%)	7 (6%)	2 (2%)	7 27
53	u	92/101 (91%)	78 (85%)	13 (14%)	1 (1%)	12 37
54	v	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	11 35
55	w	80/82 (98%)	71 (89%)	9 (11%)	0	100 100
56	x	78/84 (93%)	67 (86%)	10 (13%)	1 (1%)	10 33
57	y	53/75 (71%)	48 (91%)	5 (9%)	0	100 100
58	z	77/92 (84%)	70 (91%)	7 (9%)	0	100 100
All	All	5864/6342 (92%)	5255 (90%)	585 (10%)	24 (0%)	32 60

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	G	48	ASN
18	L	82	LEU
36	d	32	ILE
52	t	67	GLY
1	0	69	LYS

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	0	65/66 (98%)	65 (100%)	0	100	100
2	1	44/61 (72%)	43 (98%)	1 (2%)	45	67
6	6	59/62 (95%)	58 (98%)	1 (2%)	56	74
9	C	216/218 (99%)	215 (100%)	1 (0%)	86	91
10	D	164/164 (100%)	164 (100%)	0	100	100
11	E	165/165 (100%)	165 (100%)	0	100	100
12	F	148/150 (99%)	147 (99%)	1 (1%)	81	88
13	G	137/138 (99%)	137 (100%)	0	100	100
14	H	38/114 (33%)	38 (100%)	0	100	100
15	I	109/110 (99%)	106 (97%)	3 (3%)	38	62
16	J	116/116 (100%)	116 (100%)	0	100	100
17	K	103/104 (99%)	103 (100%)	0	100	100
18	L	102/103 (99%)	101 (99%)	1 (1%)	73	83
19	M	109/109 (100%)	109 (100%)	0	100	100
20	N	100/103 (97%)	99 (99%)	1 (1%)	73	83
21	O	86/87 (99%)	85 (99%)	1 (1%)	67	80
22	P	99/100 (99%)	99 (100%)	0	100	100
23	Q	89/90 (99%)	89 (100%)	0	100	100
24	R	84/84 (100%)	84 (100%)	0	100	100
25	S	93/93 (100%)	91 (98%)	2 (2%)	47	68
26	T	48/49 (98%)	48 (100%)	0	100	100
27	U	83/85 (98%)	82 (99%)	1 (1%)	67	80
28	V	78/78 (100%)	78 (100%)	0	100	100
29	W	56/63 (89%)	56 (100%)	0	100	100
30	X	67/68 (98%)	67 (100%)	0	100	100
31	Y	55/55 (100%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Z	83/84 (99%)	83 (100%)	0	100	100
33	a	47/48 (98%)	47 (100%)	0	100	100
34	b	45/49 (92%)	44 (98%)	1 (2%)	47	68
35	c	38/38 (100%)	38 (100%)	0	100	100
36	d	51/52 (98%)	51 (100%)	0	100	100
37	e	34/34 (100%)	33 (97%)	1 (3%)	37	61
39	g	148/149 (99%)	145 (98%)	3 (2%)	50	70
40	h	100/100 (100%)	100 (100%)	0	100	100
41	i	180/199 (90%)	177 (98%)	3 (2%)	56	74
42	j	170/190 (90%)	170 (100%)	0	100	100
43	k	172/173 (99%)	169 (98%)	3 (2%)	56	74
44	l	113/126 (90%)	112 (99%)	1 (1%)	75	86
45	m	87/116 (75%)	86 (99%)	1 (1%)	70	81
46	n	124/147 (84%)	123 (99%)	1 (1%)	79	87
47	o	104/105 (99%)	104 (100%)	0	100	100
48	p	105/107 (98%)	103 (98%)	2 (2%)	52	71
49	q	86/90 (96%)	86 (100%)	0	100	100
50	r	90/99 (91%)	88 (98%)	2 (2%)	47	68
51	s	103/104 (99%)	102 (99%)	1 (1%)	73	83
52	t	92/96 (96%)	92 (100%)	0	100	100
53	u	79/84 (94%)	79 (100%)	0	100	100
54	v	75/77 (97%)	75 (100%)	0	100	100
55	w	65/65 (100%)	65 (100%)	0	100	100
56	x	74/78 (95%)	73 (99%)	1 (1%)	62	77
57	y	48/65 (74%)	48 (100%)	0	100	100
58	z	70/79 (89%)	70 (100%)	0	100	100
All	All	4896/5189 (94%)	4863 (99%)	33 (1%)	80	88

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	p	45	ARG
50	r	106	ARG

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Mol	Chain	Res	Type
56	x	77	ARG
27	U	7	ARG
25	S	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
31	Y	25	GLN
41	i	89	GLN
31	Y	27	ASN
33	a	42	HIS
46	n	28	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	58/73 (79%)	13 (22%)	1 (1%)
38	f	1538/1539 (99%)	262 (17%)	0
4	3	63/77 (81%)	7 (11%)	0
5	4	58/76 (76%)	17 (29%)	1 (1%)
7	A	2902/2903 (99%)	477 (16%)	7 (0%)
8	B	117/118 (99%)	14 (11%)	0
All	All	4736/4786 (98%)	790 (16%)	9 (0%)

5 of 790 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	13	C
3	2	14	A
3	2	15	G
3	2	19	G
3	2	20	G

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	2146	C
7	A	2428	G
7	A	404	A
7	A	479	A

Continued on next page...

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Mol	Chain	Res	Type
7	A	885	C

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

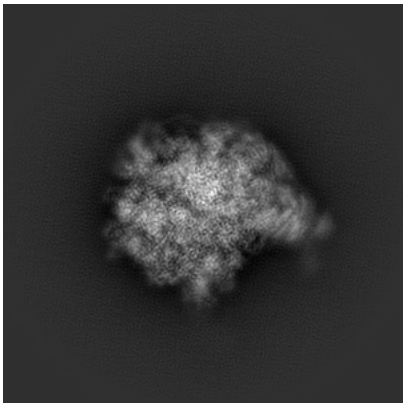
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30598. These allow visual inspection of the internal detail of the map and identification of artifacts.

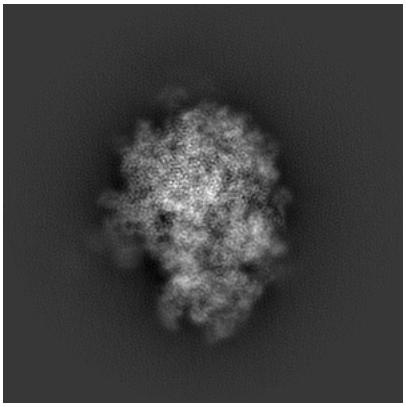
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

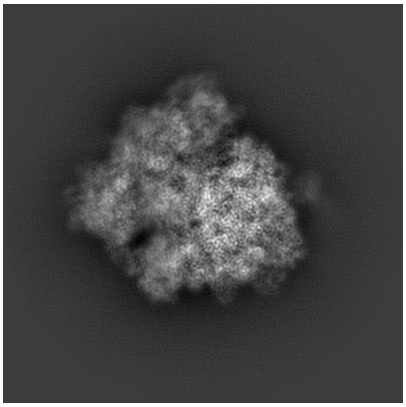
6.1.1 Primary map



X



Y

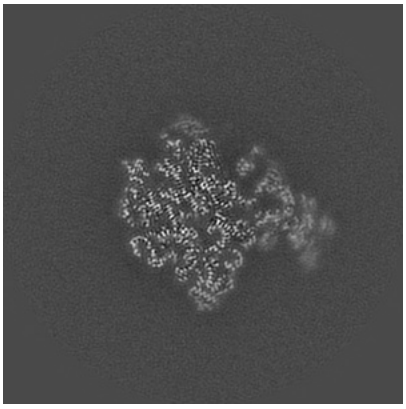


Z

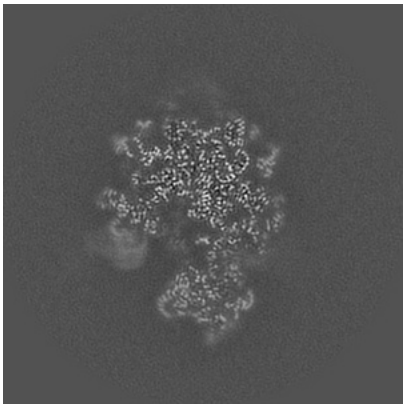
The images above show the map projected in three orthogonal directions.

6.2 Central slices

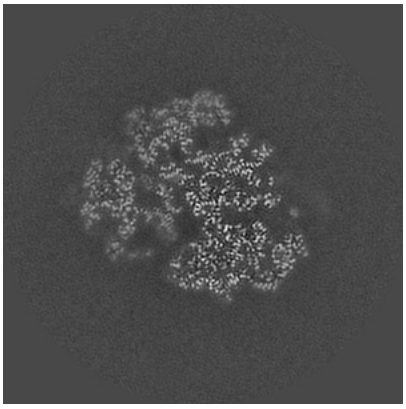
6.2.1 Primary map



X Index: 160



Y Index: 160

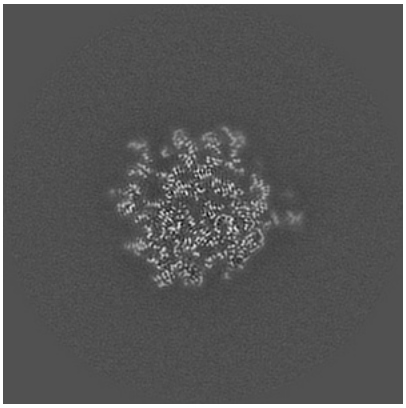


Z Index: 160

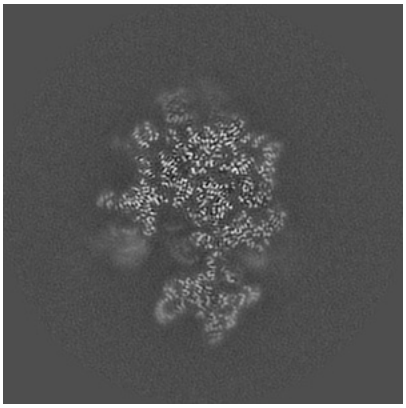
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

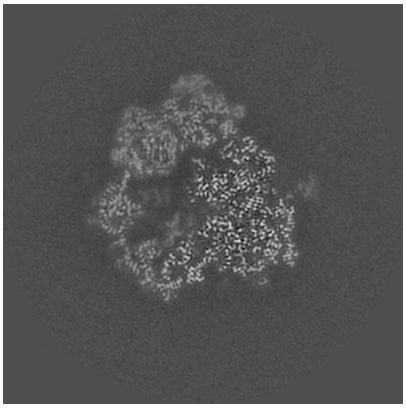
6.3.1 Primary map



X Index: 186



Y Index: 165

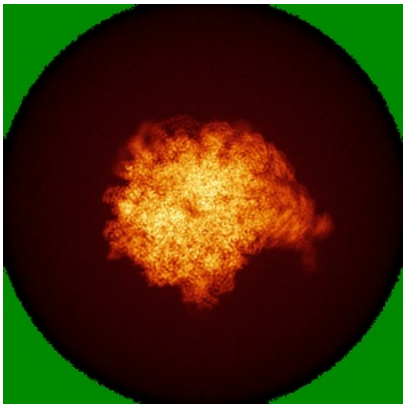


Z Index: 146

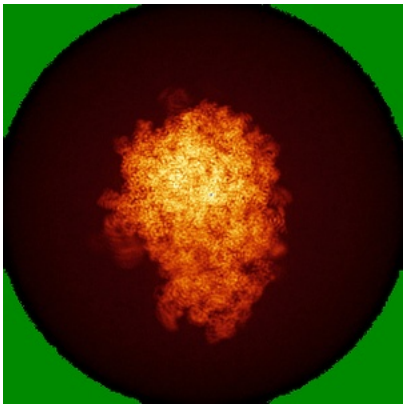
The images above show the largest variance slices of the map in three orthogonal directions.

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

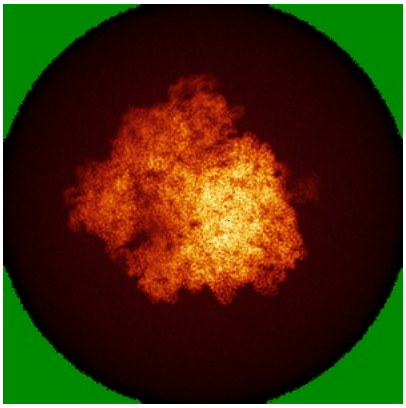
6.4.1 Primary map



X



Y



Z

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

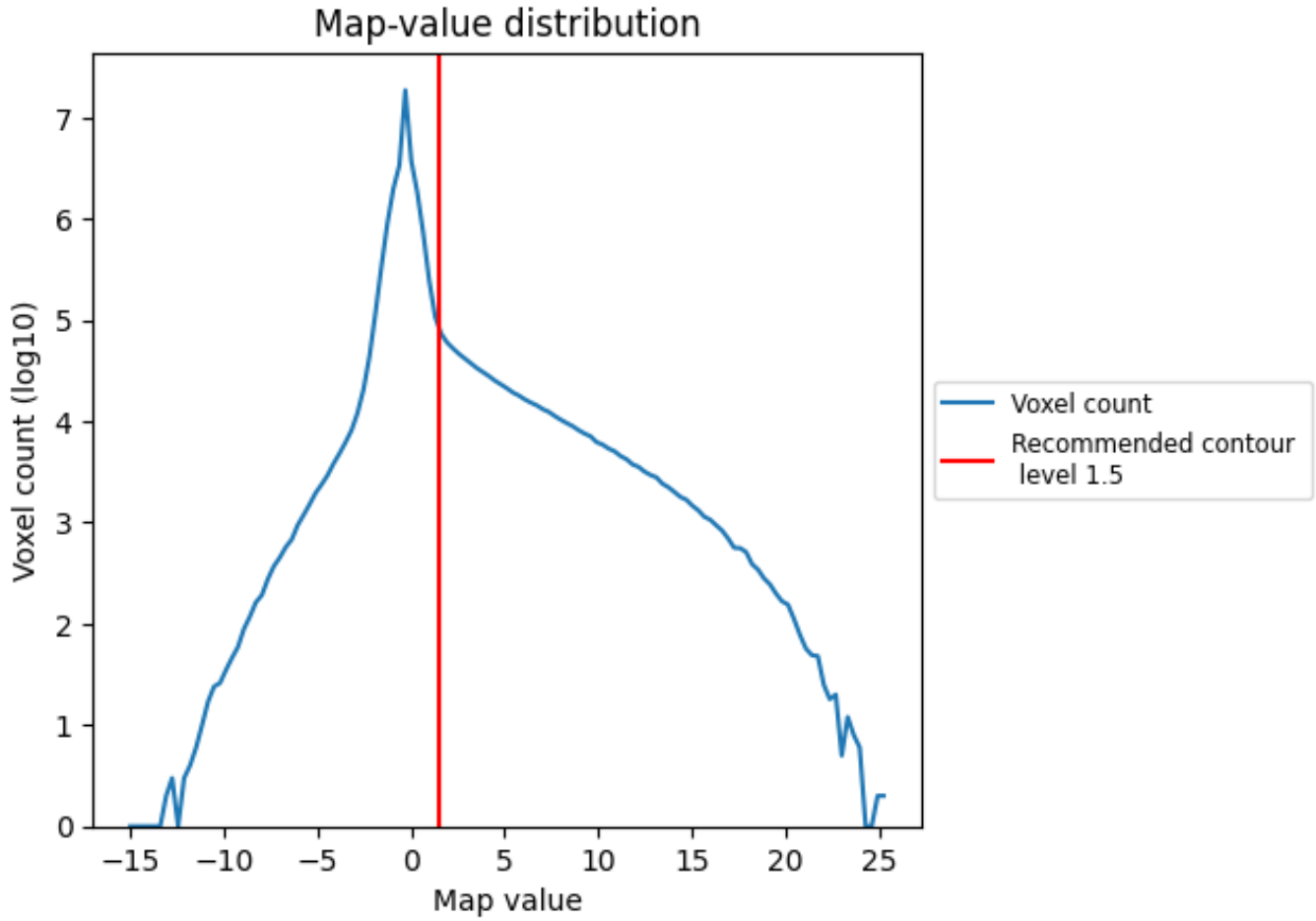
6.6 Mask visualisation (i)

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

7 Map analysis

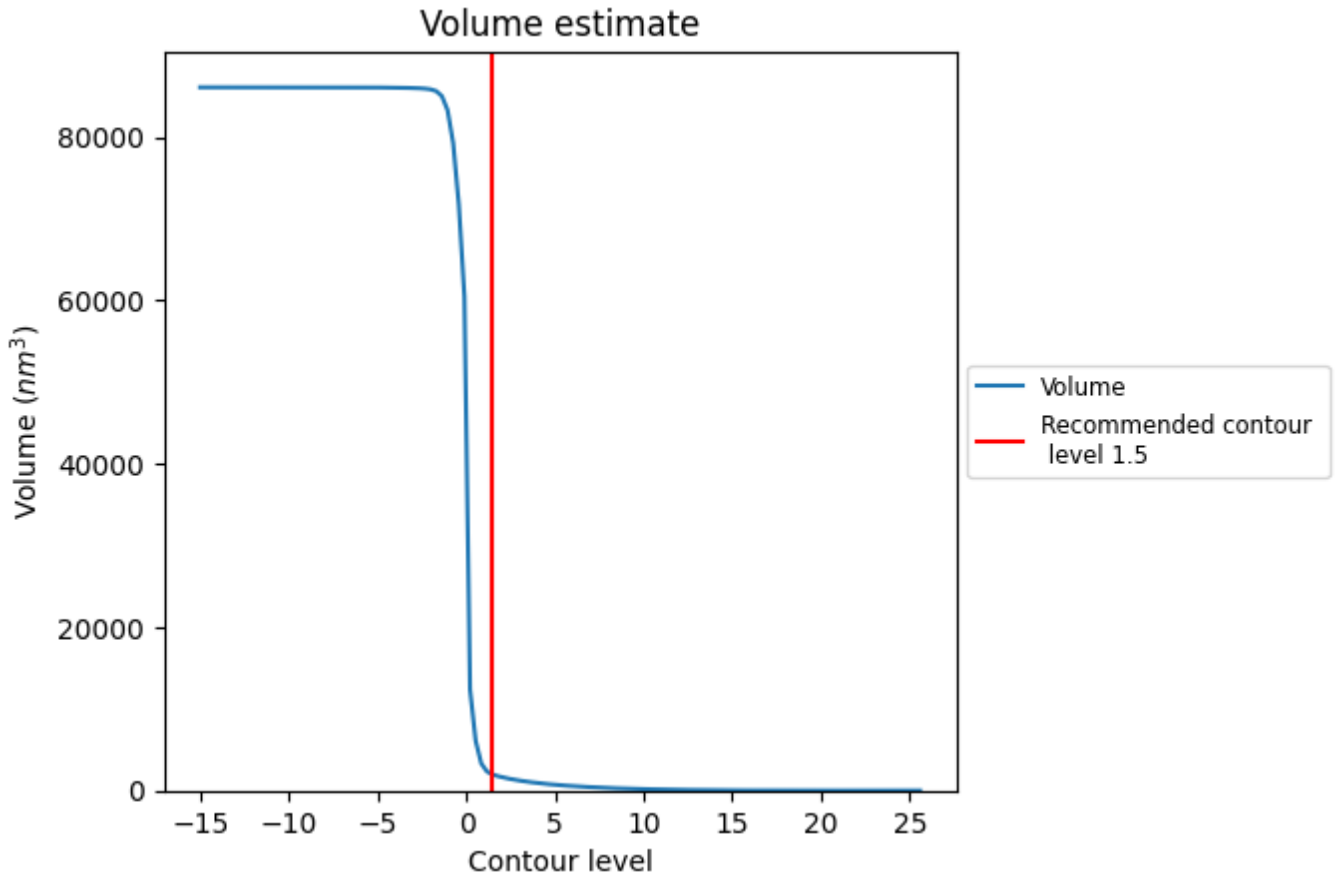
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

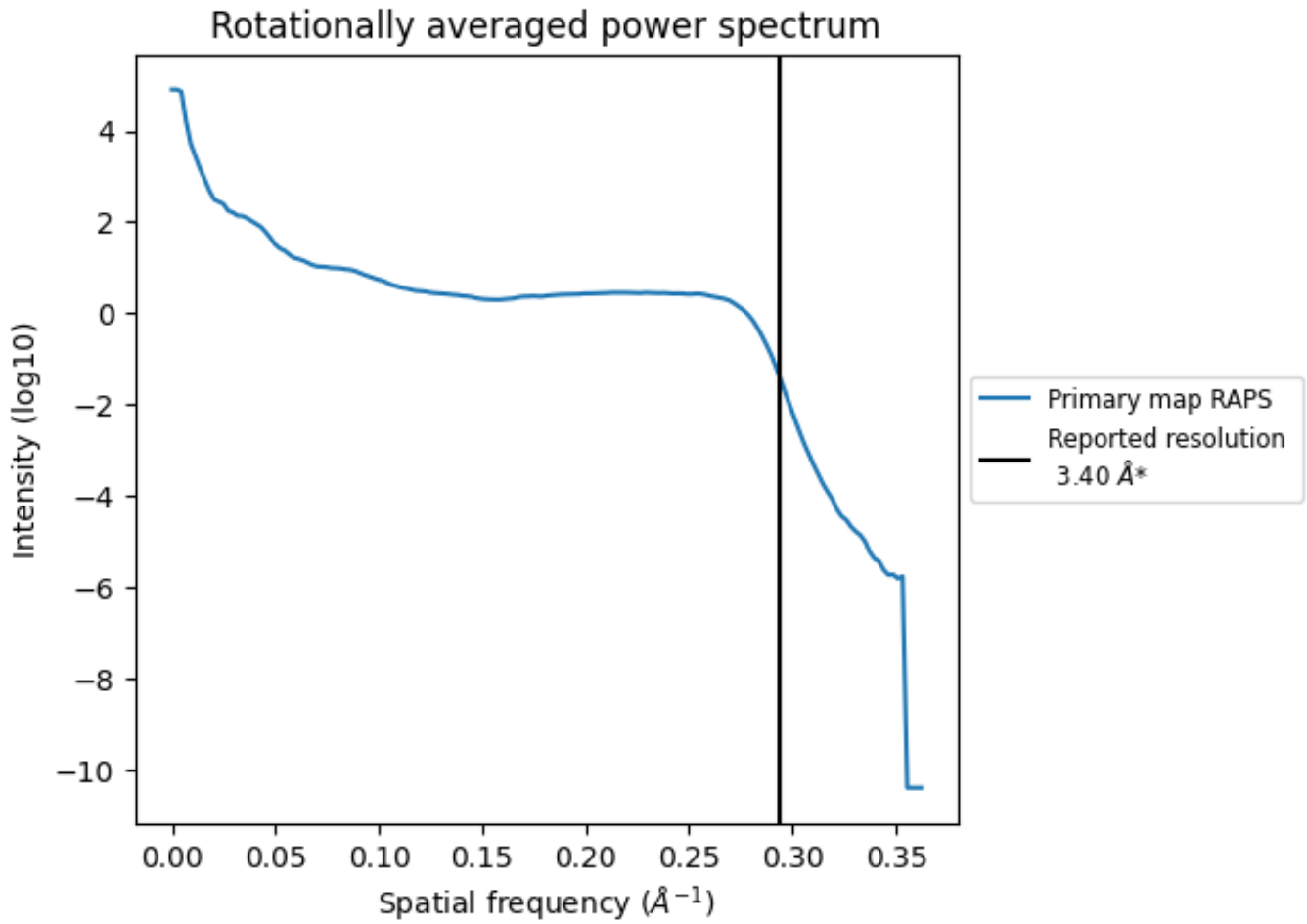
7.2 Volume estimate (i)



The volume at the recommended contour level is 1962 nm^3; this corresponds to an approximate mass of 1772 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)

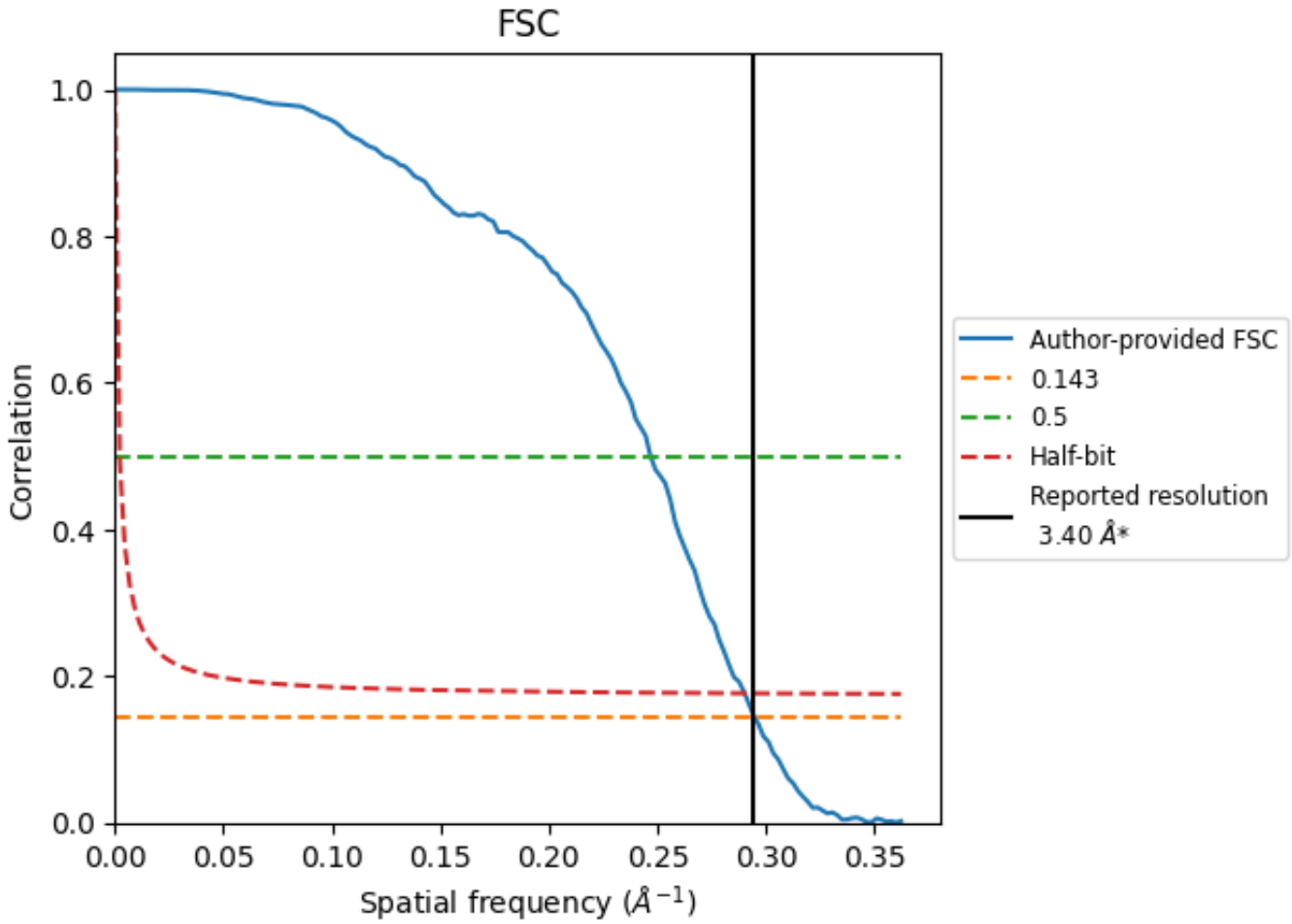


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

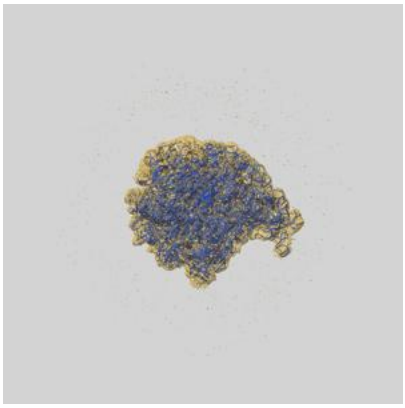
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	4.05	3.45
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

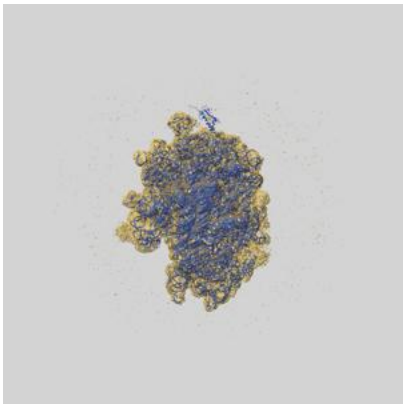
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30598 and PDB model 7D6Z. Per-residue inclusion information can be found in section 3 on page 15.

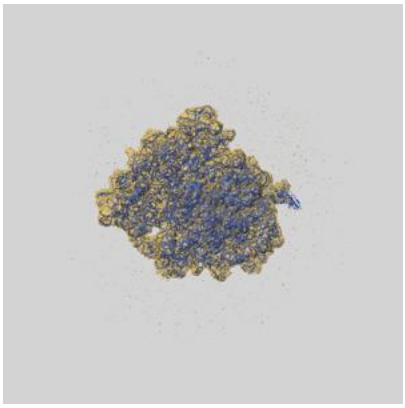
9.1 Map-model overlay



X



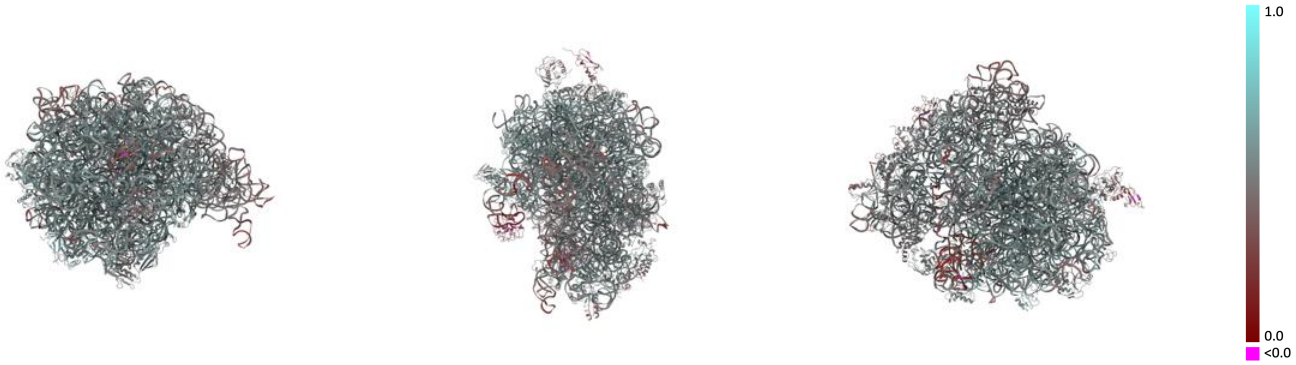
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5 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.

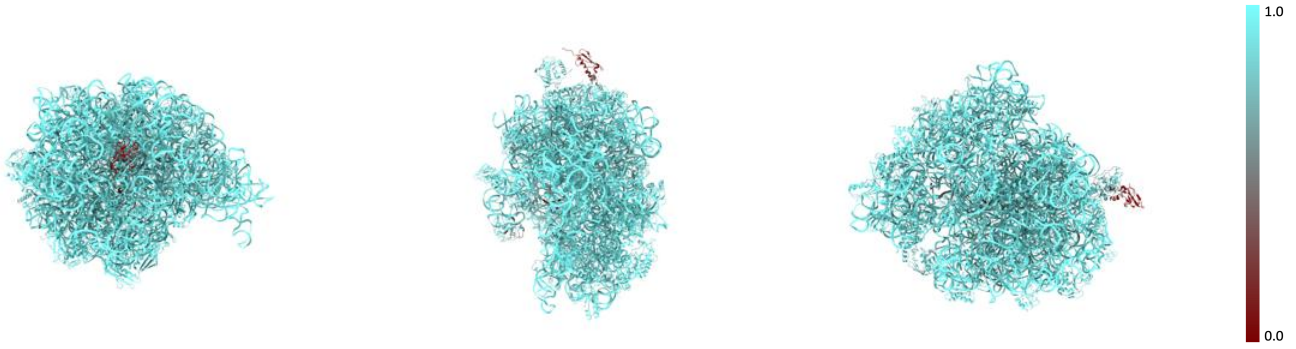
9.2 Q-score mapped to coordinate model



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.

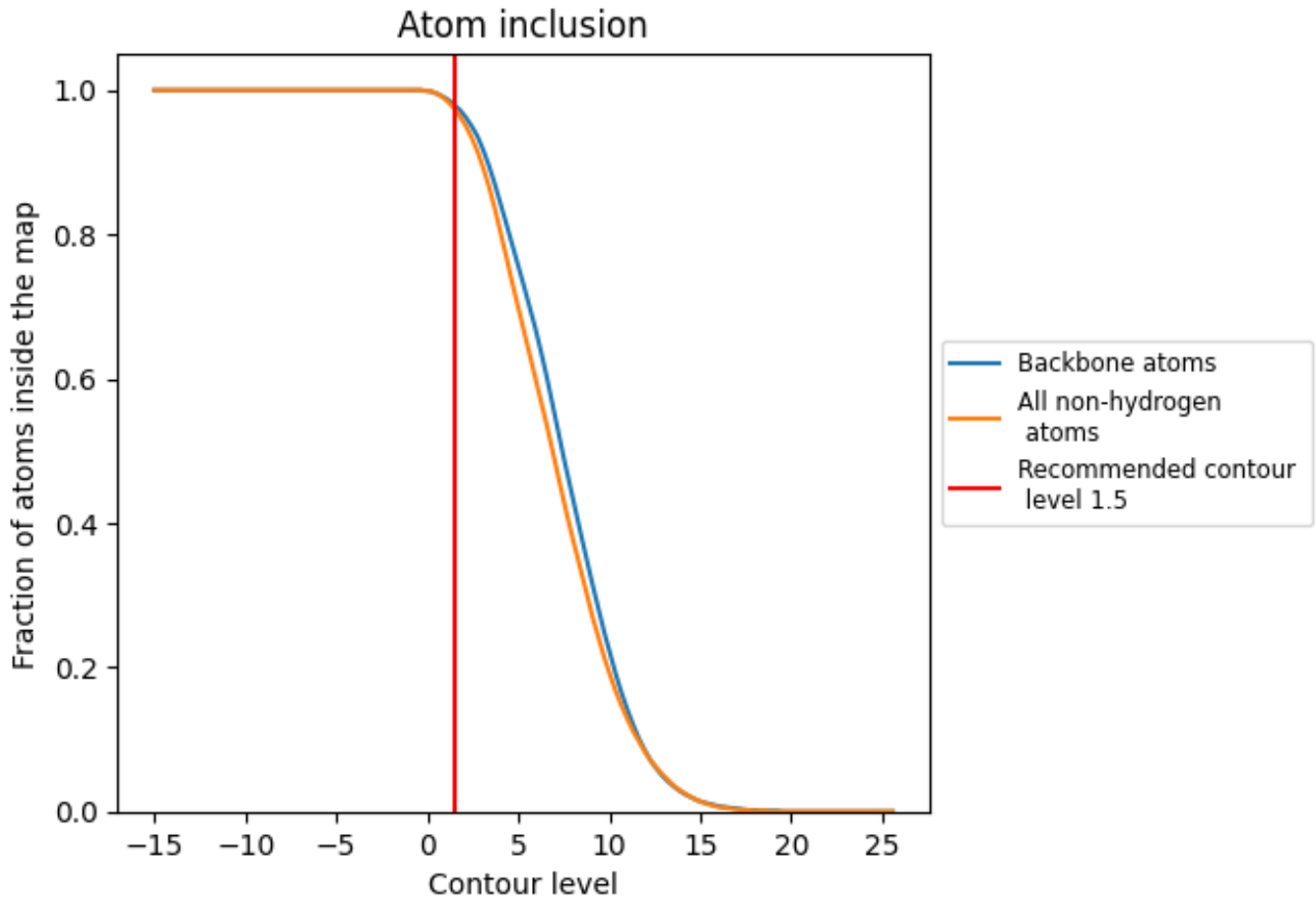
9.3 Atom inclusion mapped to coordinate model



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 (1.5).

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

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9740	0.5050
0	0.9680	0.4600
1	0.8500	0.4020
2	0.9540	0.3200
3	0.9630	0.4720
4	0.3710	0.3900
6	0.7260	0.4510
A	0.9960	0.5210
B	0.9980	0.5200
C	0.9820	0.5700
D	0.9810	0.5600
E	0.9880	0.5520
F	0.9760	0.4950
G	0.9820	0.5180
H	0.9690	0.5040
I	0.7500	0.2130
J	0.9840	0.5670
K	0.9760	0.5520
L	0.9790	0.5560
M	0.9840	0.5660
N	0.9910	0.5640
O	0.9910	0.5330
P	0.9730	0.5540
Q	0.9920	0.5660
R	0.9750	0.5520
S	0.9640	0.5570
T	0.9790	0.5520
U	0.9820	0.5290
V	0.9840	0.5490
W	0.9820	0.5760
X	0.9850	0.5640
Y	0.9560	0.5140
Z	0.9610	0.5170
a	0.9670	0.5610
b	0.9100	0.5480

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Chain	Atom inclusion	Q-score
c	0.9750	0.5740
d	0.9820	0.5840
e	0.9900	0.5670
f	0.9970	0.4880
g	0.8380	0.4190
h	0.2200	0.3370
i	0.9670	0.4670
j	0.9730	0.5140
k	0.9420	0.3810
l	0.9730	0.5250
m	0.9640	0.4830
n	0.9730	0.4870
o	0.9720	0.5260
p	0.9700	0.4720
q	0.9760	0.4610
r	0.9770	0.5160
s	0.9450	0.4750
t	0.9790	0.4810
u	0.9740	0.4900
v	0.9750	0.5080
w	0.9410	0.4790
x	0.9590	0.4680
y	0.9860	0.5290
z	0.9740	0.5000