wwPDB EM Validation Summary Report

Mar 12, 2025 – 10:13 AM EDT

PDB ID	:	9MQ4
EMDB ID	:	EMD-48513
Title	:	Damaged 70S ribosome with PrfH bound
Authors	:	Tian, Y.; Li, Q.; Jin, H.; Fatma, S.; Zeng, F.; Huang, R.H.
Deposited on	:	2025-01-01
Resolution	:	2.78 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:

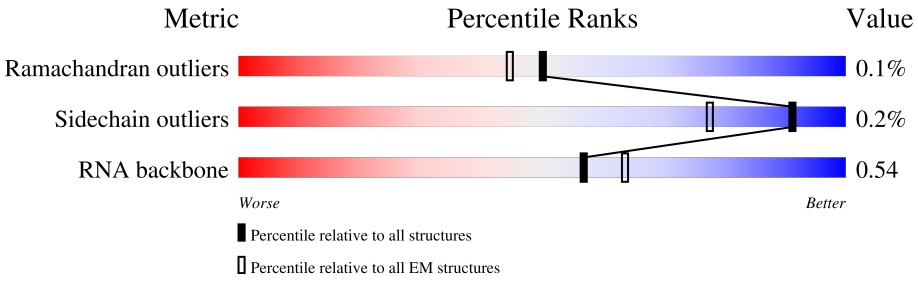
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.78 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	1	2903	10% 81% 19%
2	2	1534	14% 81% 19%
3	4	120	5% 82% 18%
4	5	77	25% 77% 23%
4	6	77	99% 78% 22%
5	7	25	20% 76%
6	A	231	88% 98%
7	B	273	7% 99%

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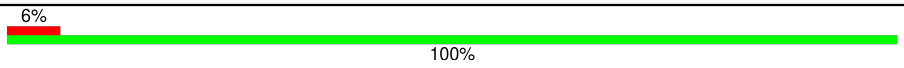
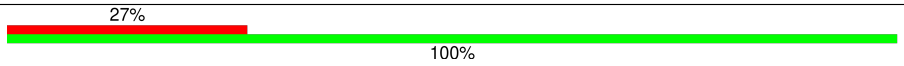
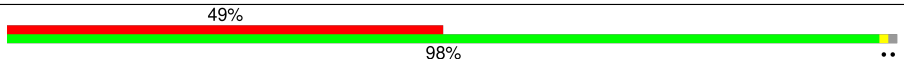
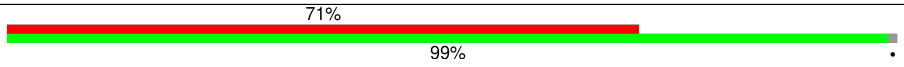
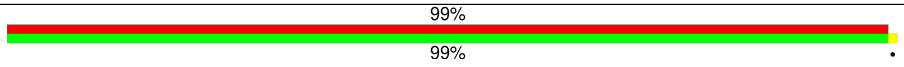
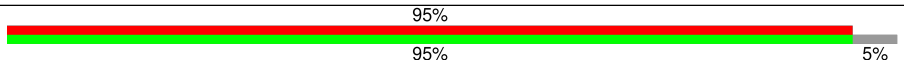
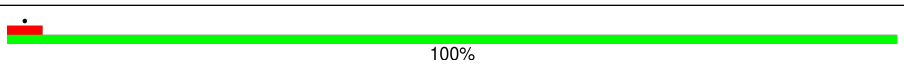
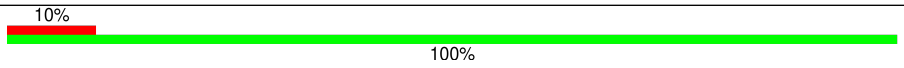
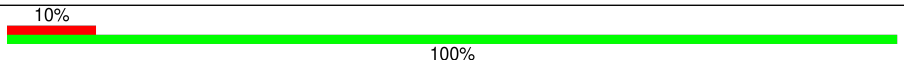
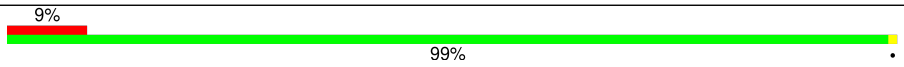
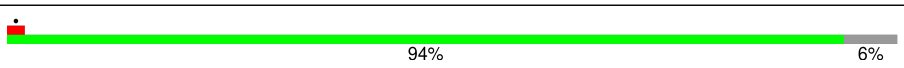
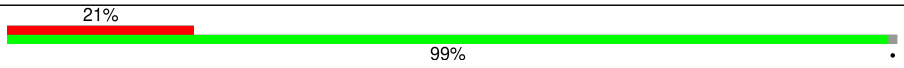
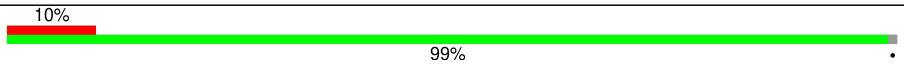
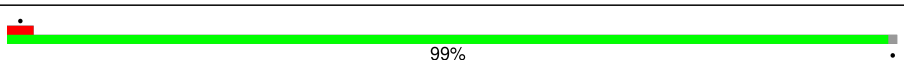
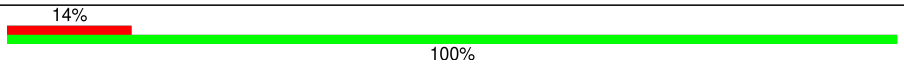
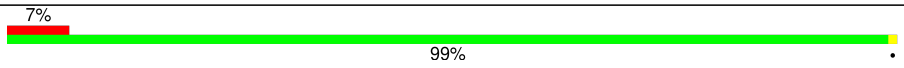
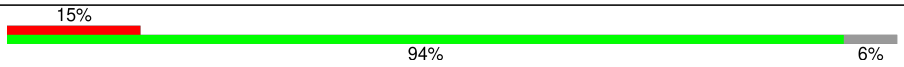
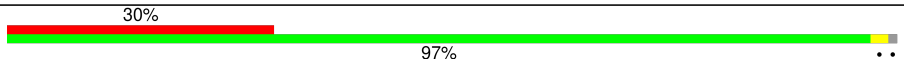
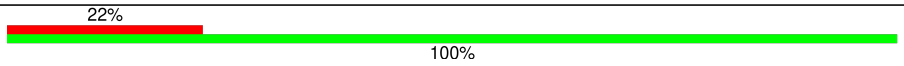
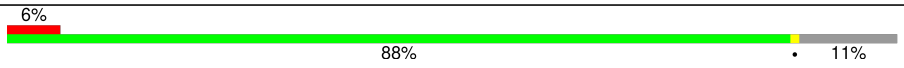
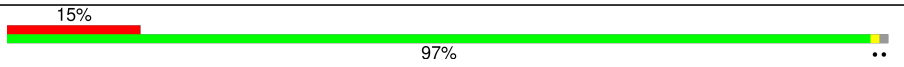
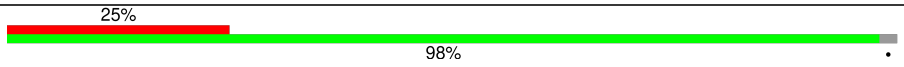
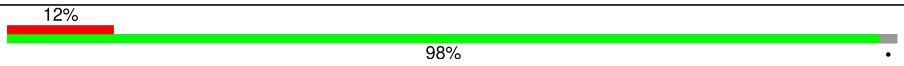
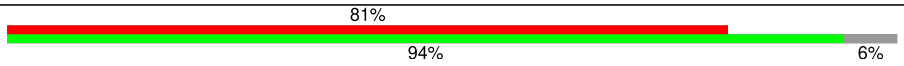
Mol	Chain	Length	Quality of chain
8	C	209	
9	D	201	
10	E	179	
11	F	177	
12	G	149	
13	H	165	
14	I	142	
15	J	142	
16	K	123	
17	L	144	
18	M	136	
19	N	127	
20	O	117	
21	P	115	
22	Q	118	
23	R	103	
24	S	110	
25	T	100	
26	U	104	
27	V	94	
28	W	85	
29	X	78	
30	Y	63	
31	Z	59	
32	a	70	

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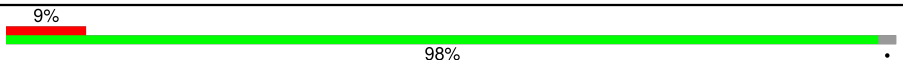
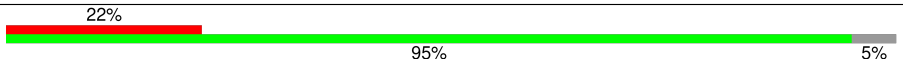
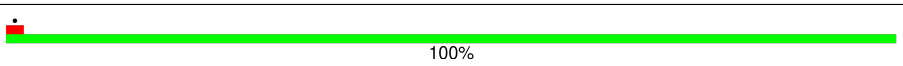
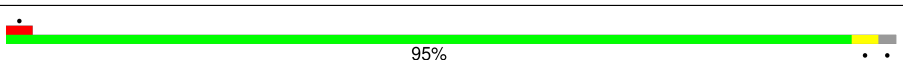
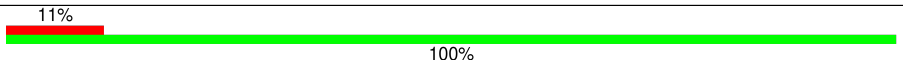
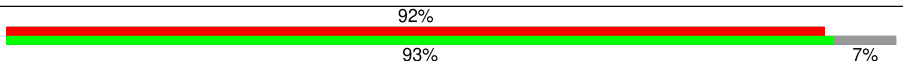
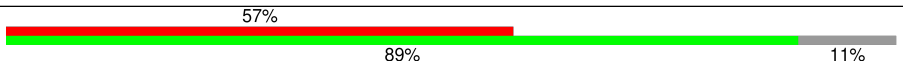
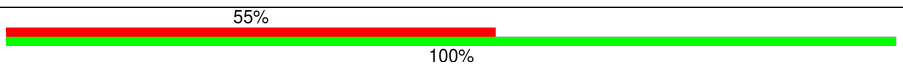
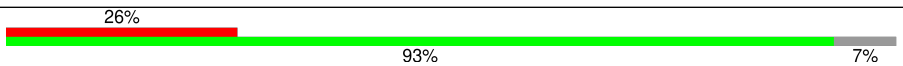
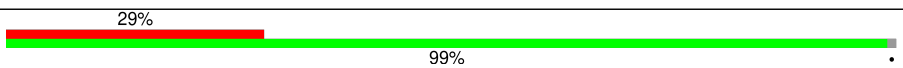
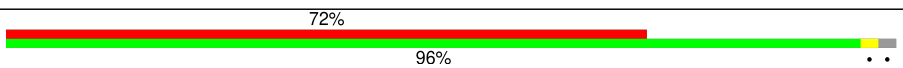
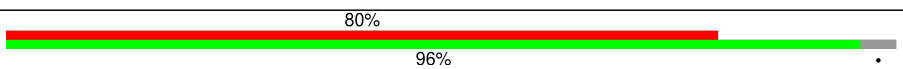
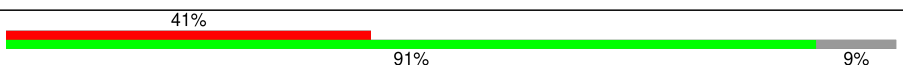
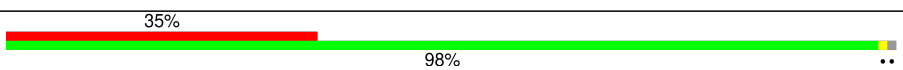
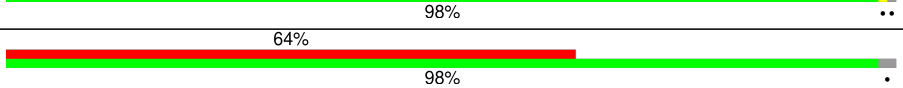
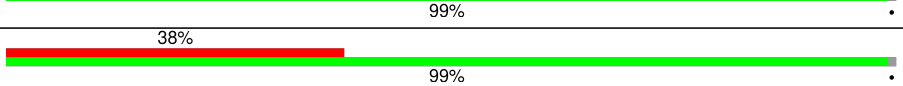
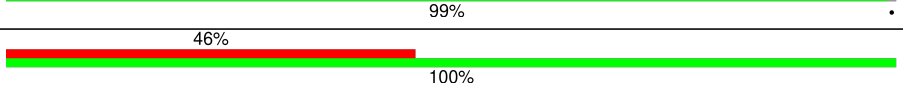
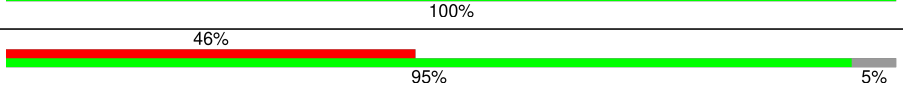
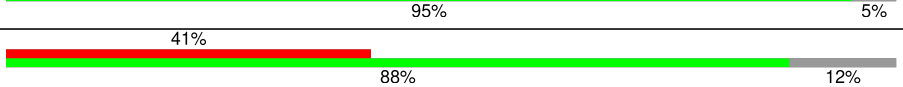
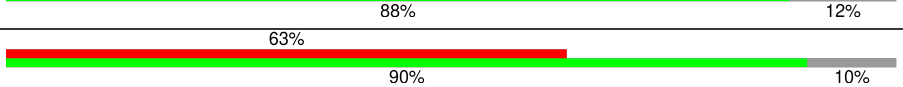
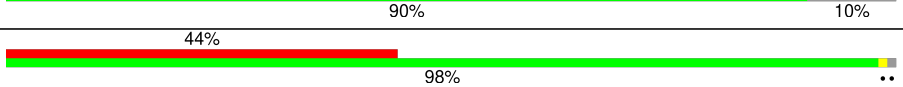
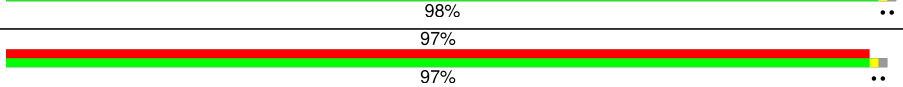
Mol	Chain	Length	Quality of chain
33	b	57	
34	c	55	
35	d	46	
36	e	65	
37	f	38	
38	g	241	
39	h	233	
40	i	206	
41	j	167	
42	k	135	
43	l	179	
44	m	130	
45	n	130	
46	o	103	
47	p	129	
48	q	124	
49	r	118	
50	s	101	
51	t	89	
52	u	82	
53	v	84	
54	w	75	
55	x	92	
56	y	87	
57	z	71	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	1	2069	X	-	-	-

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 150154 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2903	62336	27816	11470	20147	2903	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1534	32929	14693	6041	10661	1534	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	4	120	2569	1144	468	837	120	0	0

- Molecule 4 is a RNA chain called P-tRNA, E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	5	77	1643	732	297	537	77	0	0
4	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 5 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	7	6	131	59	27	39	6	0	0

- Molecule 6 is a protein called Peptide chain release factor H.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	229	Total	C	N	O	S	0	0
			1840	1157	337	342	4		

- Molecule 7 is a protein called 50S ribosomal protein L2.

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

- Molecule 8 is a protein called 50S ribosomal protein L3.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 12 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 13 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 14 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

- Molecule 15 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 17 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 18 is a protein called 50S ribosomal protein L16.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 20 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 21 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 22 is a protein called 50S ribosomal protein L20.

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

- Molecule 23 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 25 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	94	Total 746	C 470	N 140	O 134	S 2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	103	Total 788	C 498	N 148	O 142	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 28 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 29 is a protein called 50S ribosomal protein L28.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 31 is a protein called 50S ribosomal protein L30.

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

- Molecule 32 is a protein called 50S ribosomal protein L31.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	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	c	52	Total	C	N	O	0	0
			426	275	78	73		

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

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

- Molecule 38 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 39 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 40 is a protein called 30S ribosomal protein S4.

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

- Molecule 41 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 42 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 43 is a protein called 30S ribosomal protein S7.

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

- Molecule 44 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 45 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 46 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 47 is a protein called 30S ribosomal protein S11.

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

- Molecule 48 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 49 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 50 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 51 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 52 is a protein called 30S ribosomal protein S16.

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

- Molecule 53 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 54 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 55 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	x	83	Total 663	C 424	N 126	O 111	S 2	0	0

- Molecule 56 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	y	86	Total 669	C 414	N 138	O 114	S 3	0	0

- Molecule 57 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	z	70	Total 589	C 366	N 125	O 97	S 1	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	1	292	Total 292	Mg 292	0
58	2	125	Total 125	Mg 125	0
58	4	8	Total 8	Mg 8	0
58	5	5	Total 5	Mg 5	0
58	A	2	Total 2	Mg 2	0
58	C	1	Total 1	Mg 1	0
58	D	1	Total 1	Mg 1	0
58	b	2	Total 2	Mg 2	0
58	f	1	Total 1	Mg 1	0
58	i	1	Total 1	Mg 1	0
58	r	1	Total 1	Mg 1	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
59	a	1	Total Zn 1 1	0
59	f	1	Total Zn 1 1	0

- Molecule 60 is water.

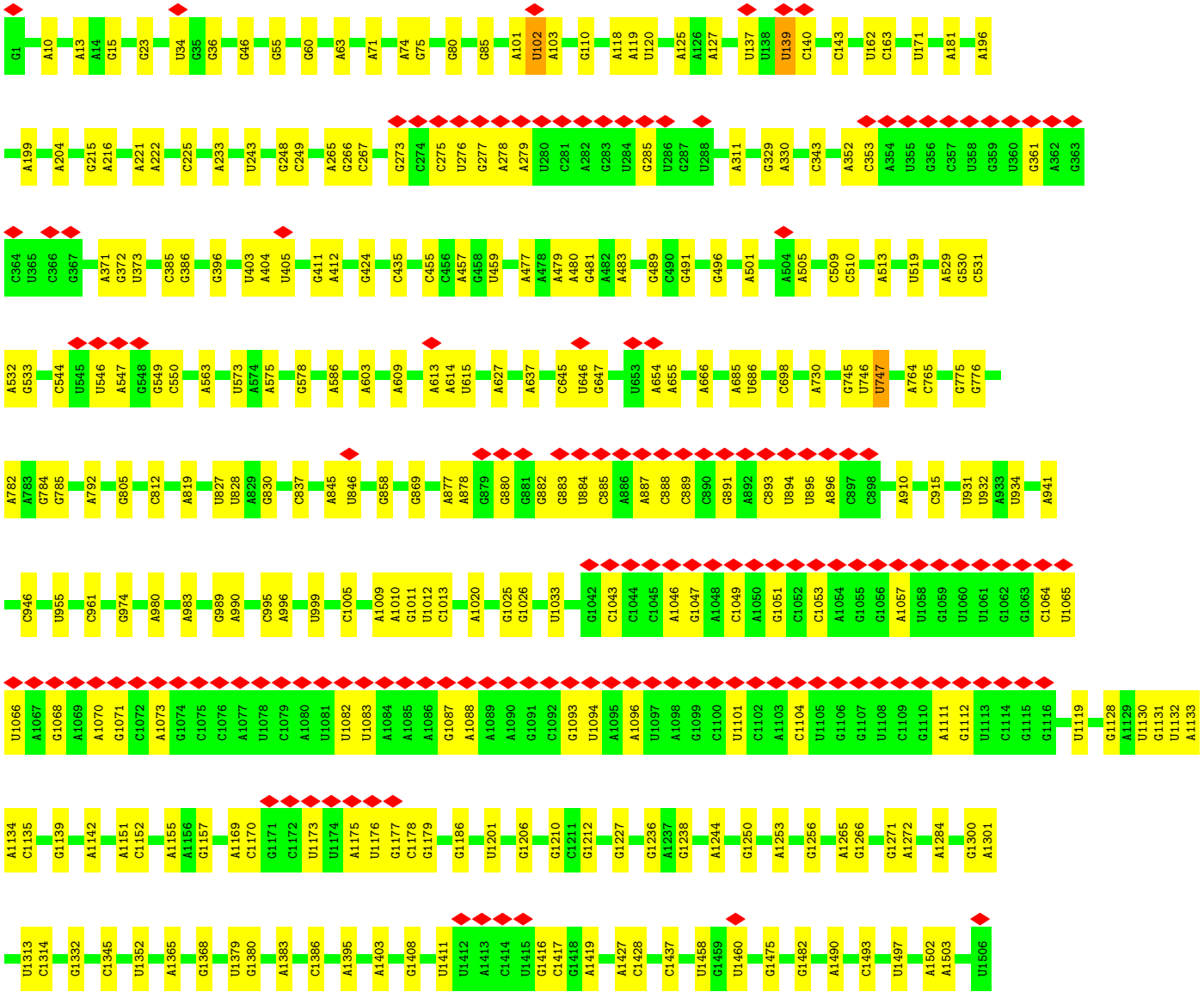
Mol	Chain	Residues	Atoms	AltConf
60	B	2	Total O 2 2	0

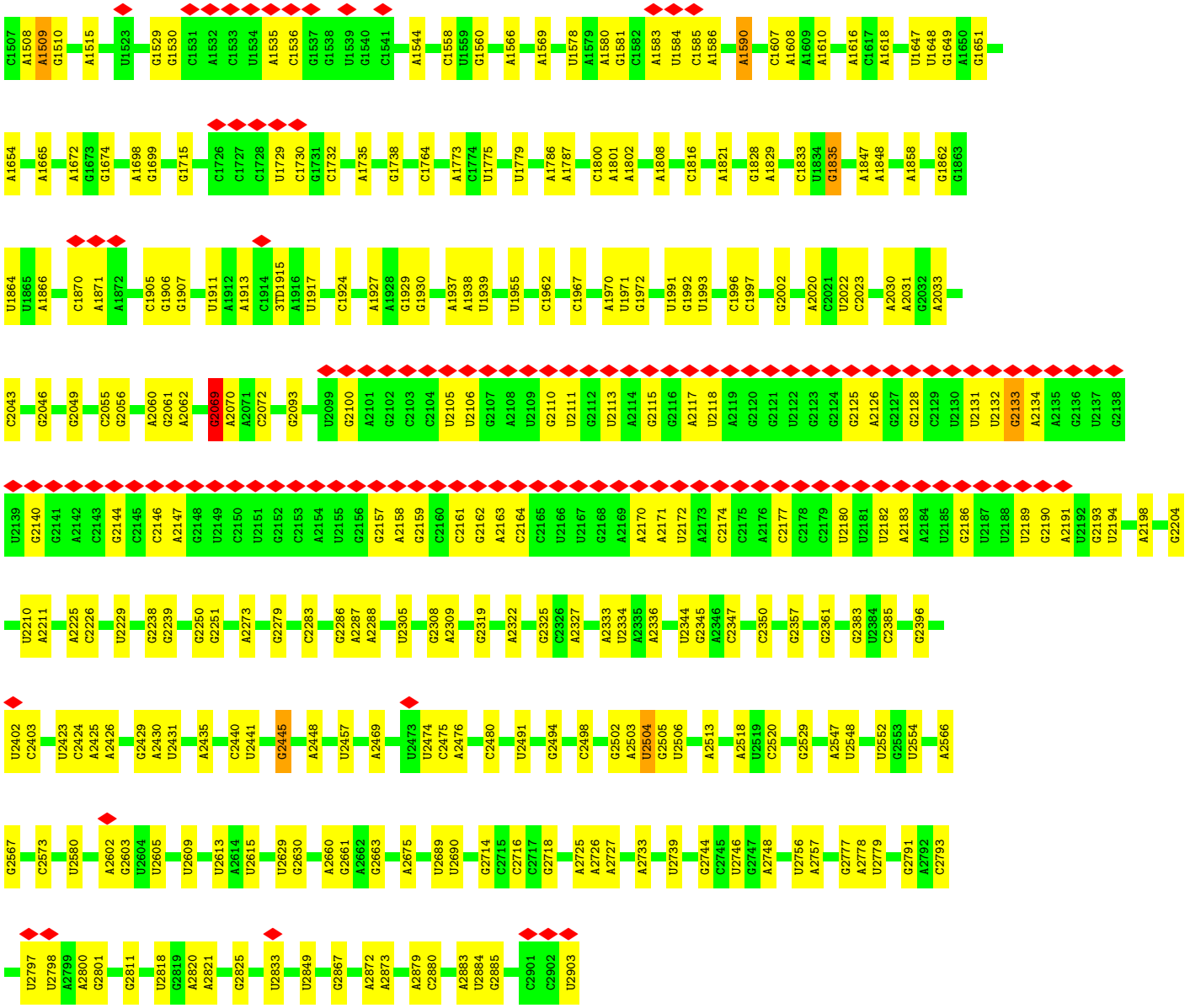
3 Residue-property plots (i)

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

- Molecule 1: 23S ribosomal RNA

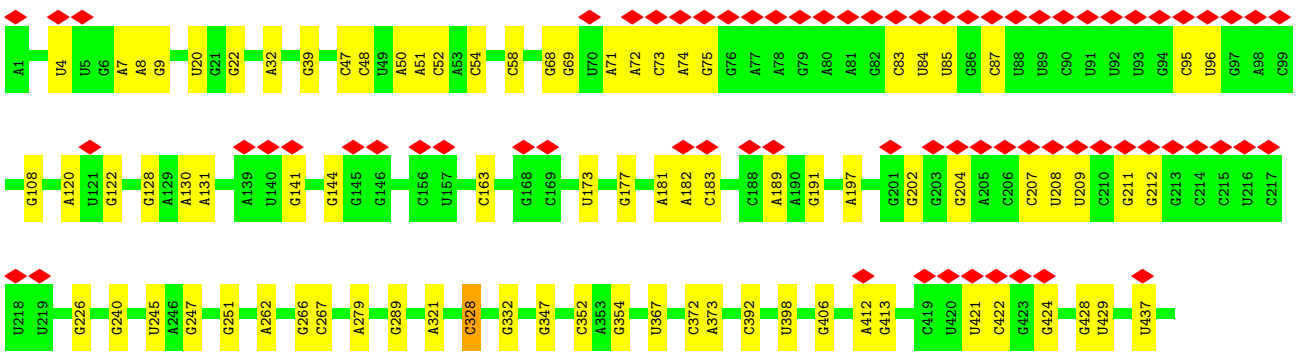
Chain 1:

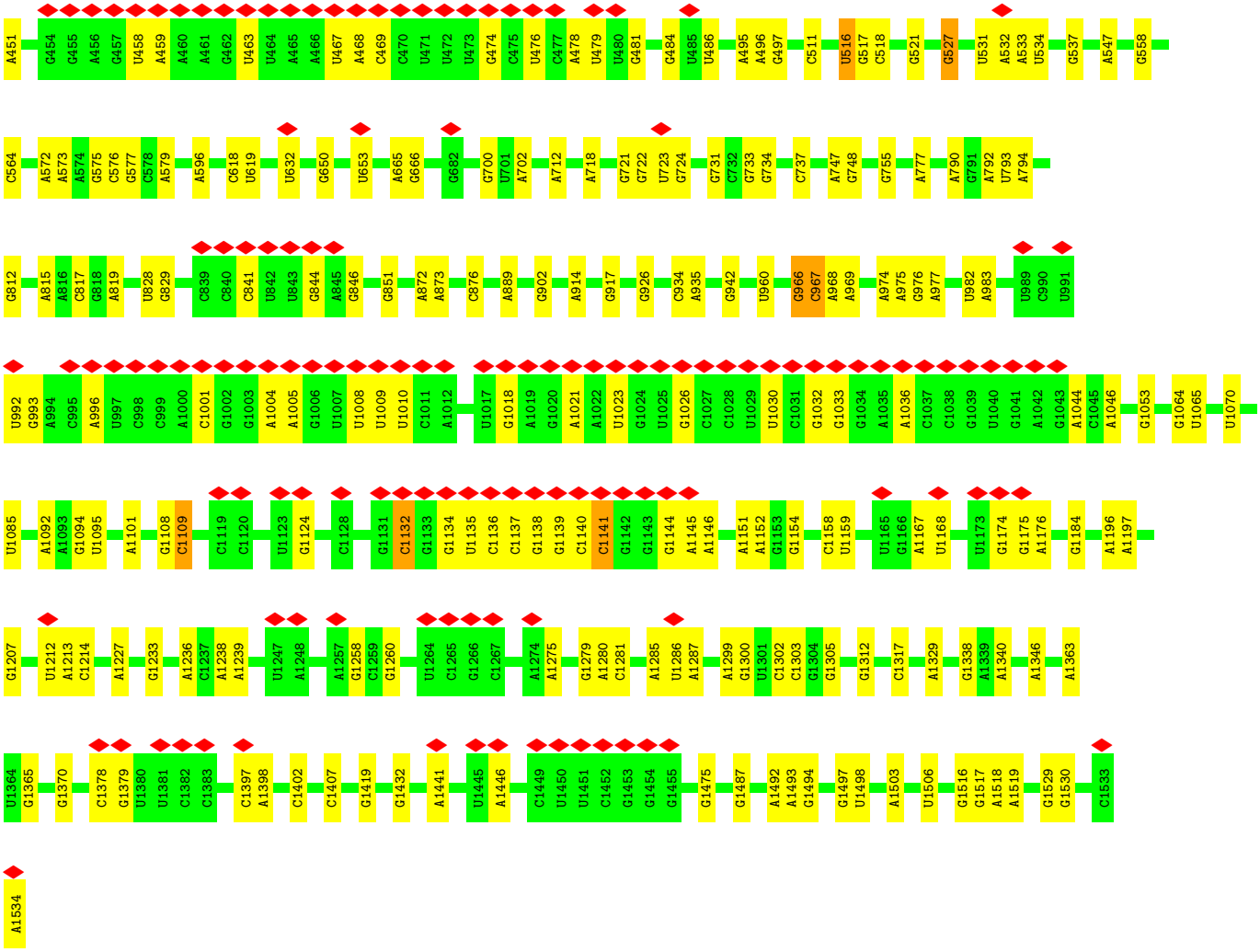




• Molecule 2: 16S ribosomal RNA

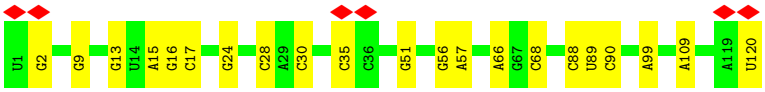
Chain 2:





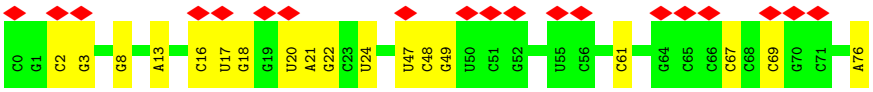
• Molecule 3: 5S ribosomal RNA

Chain 4:



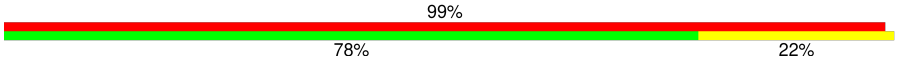
• Molecule 4: P-tRNA, E-tRNA

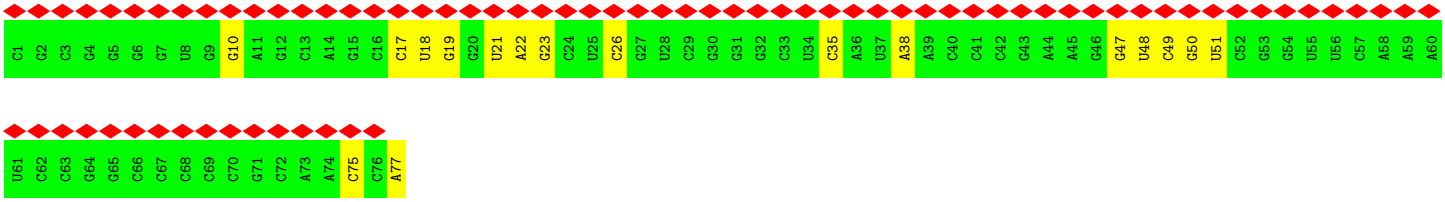
Chain 5:



• Molecule 4: P-tRNA, E-tRNA

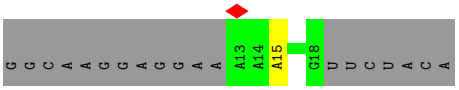
Chain 6:





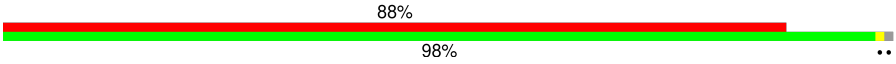
• Molecule 5: mRNA

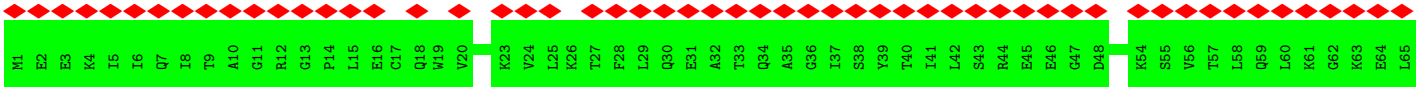
Chain 7:

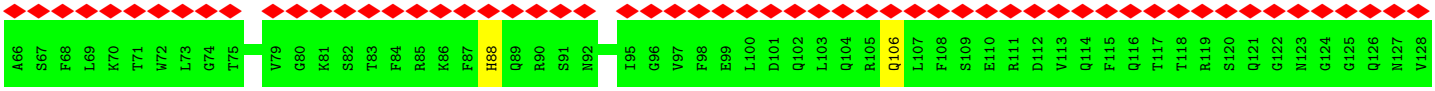


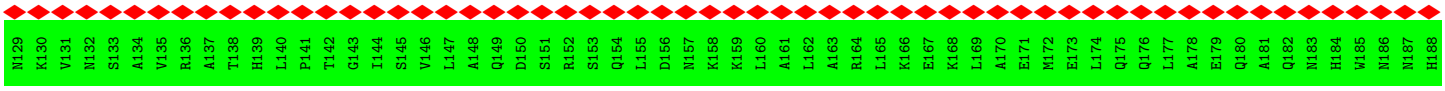
• Molecule 6: Peptide chain release factor H

Chain A:



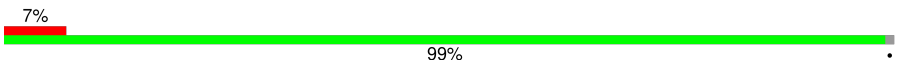


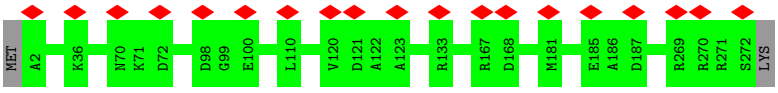




• Molecule 7: 50S ribosomal protein L2

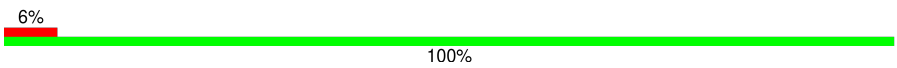
Chain B:

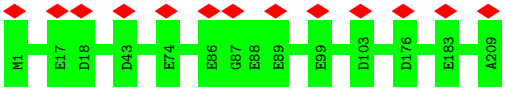




• Molecule 8: 50S ribosomal protein L3

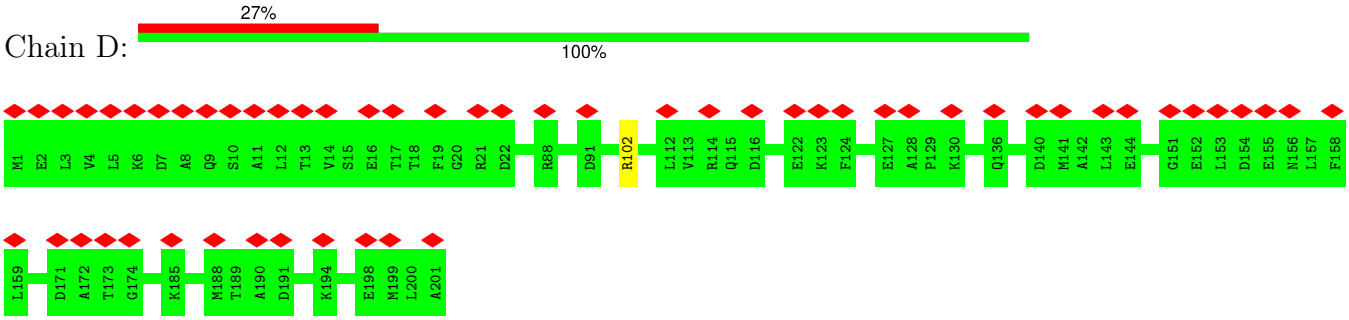
Chain C:





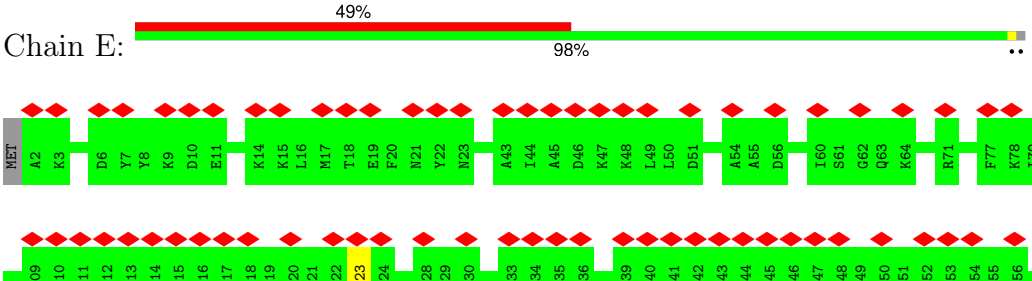
• Molecule 9: Large ribosomal subunit protein uL4

Chain D:



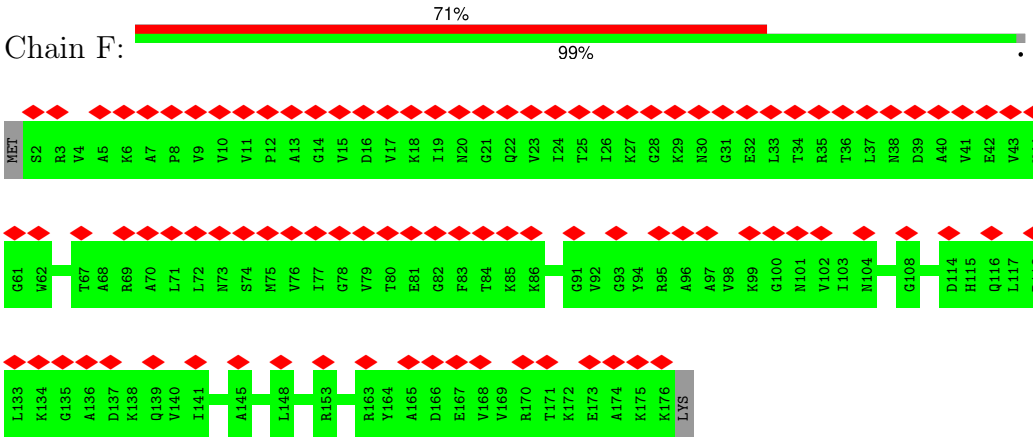
• Molecule 10: Large ribosomal subunit protein uL5

Chain E:



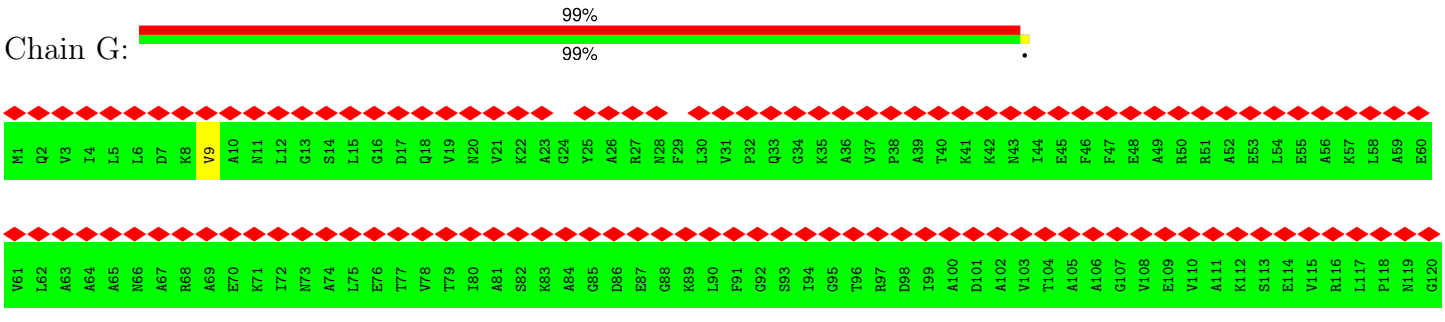
• Molecule 11: Large ribosomal subunit protein uL6

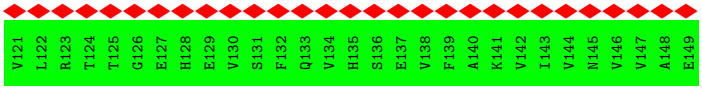
Chain F:



• Molecule 12: Large ribosomal subunit protein bL9

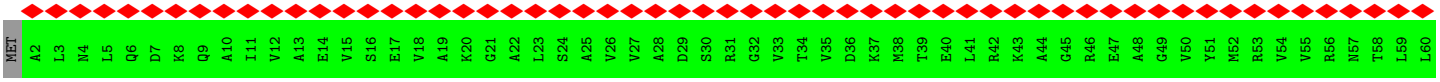
Chain G:

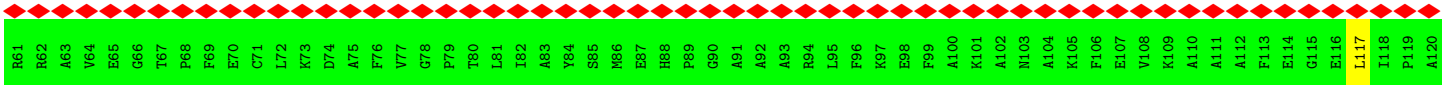


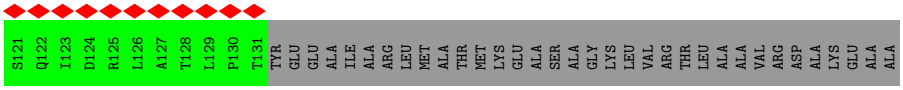


• Molecule 13: 50S ribosomal protein L10

Chain H:

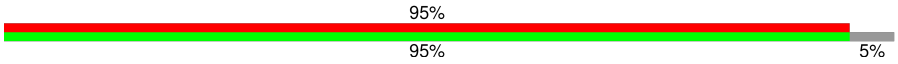


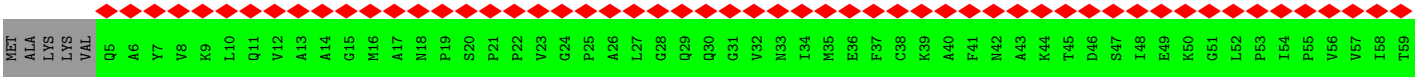


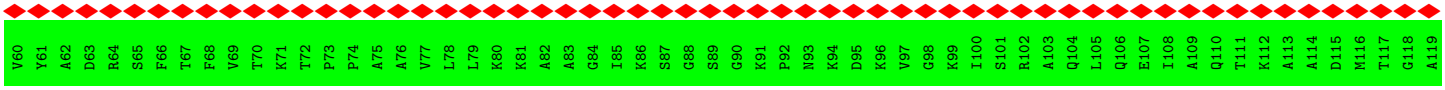


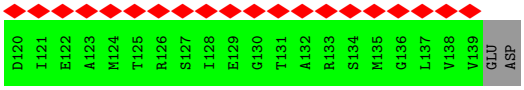
• Molecule 14: 50S ribosomal protein L11

Chain I:



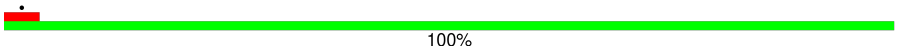


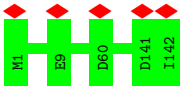




• Molecule 15: Large ribosomal subunit protein uL13

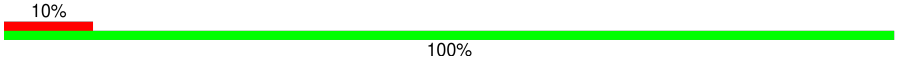
Chain J:

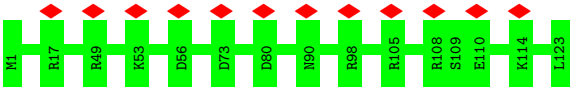




• Molecule 16: Large ribosomal subunit protein uL14

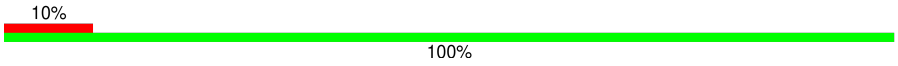
Chain K:

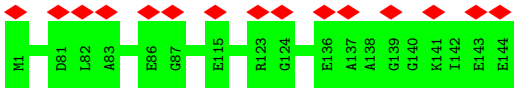




• Molecule 17: Large ribosomal subunit protein uL15

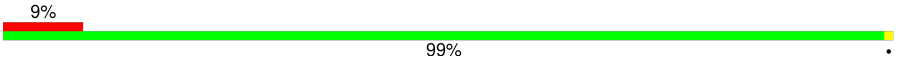
Chain L:

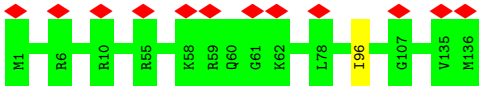




• Molecule 18: 50S ribosomal protein L16

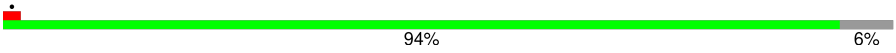
Chain M:

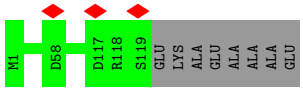




• Molecule 19: Large ribosomal subunit protein bL17

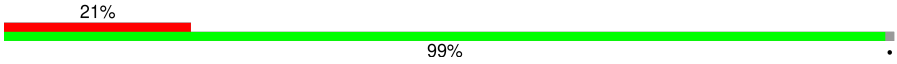
Chain N:

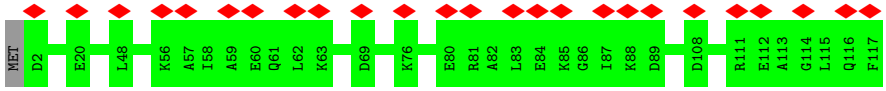




• Molecule 20: Large ribosomal subunit protein uL18

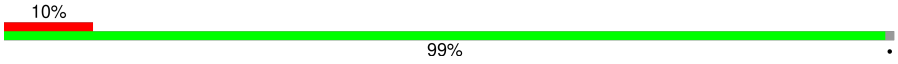
Chain O:

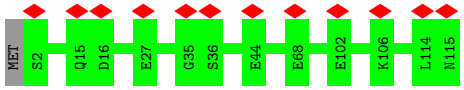




• Molecule 21: Large ribosomal subunit protein bL19

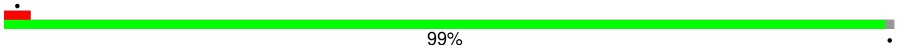
Chain P:

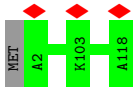




• Molecule 22: 50S ribosomal protein L20

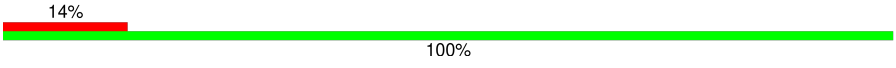
Chain Q:

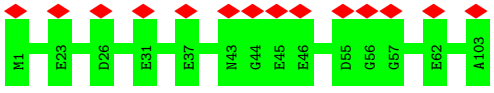




• Molecule 23: Large ribosomal subunit protein bL21

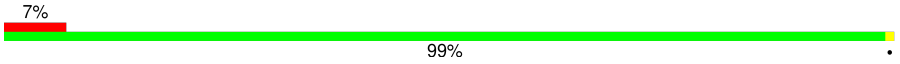
Chain R:

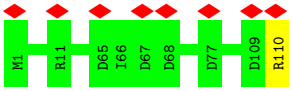




• Molecule 24: Large ribosomal subunit protein uL22

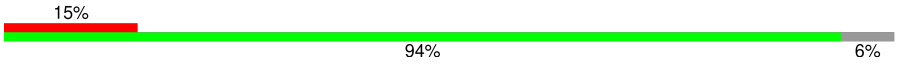
Chain S:

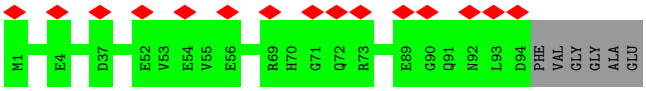




• Molecule 25: 50S ribosomal protein L23

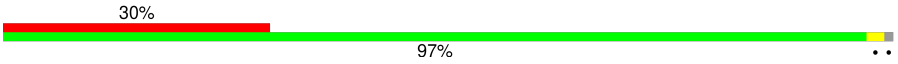
Chain T:

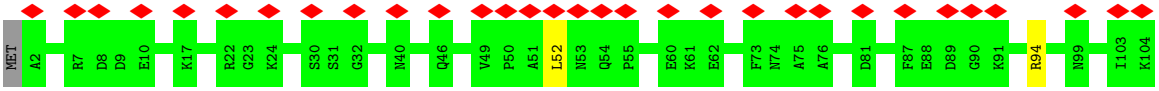




• Molecule 26: 50S ribosomal protein L24

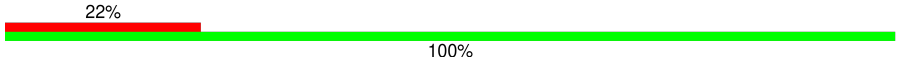
Chain U:

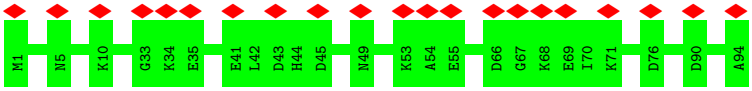




• Molecule 27: Large ribosomal subunit protein bL25

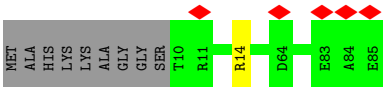
Chain V:





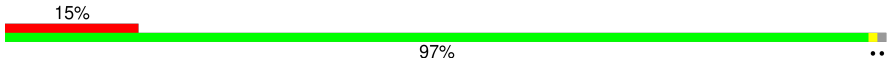
• Molecule 28: Large ribosomal subunit protein bL27

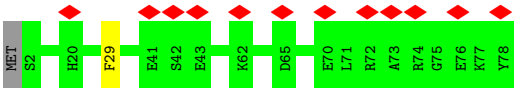
Chain W:



• Molecule 29: 50S ribosomal protein L28

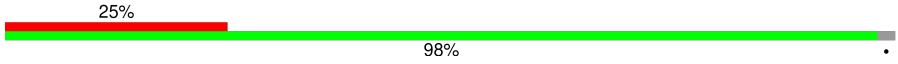
Chain X:

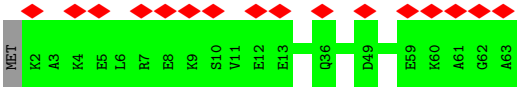




• Molecule 30: Large ribosomal subunit protein uL29

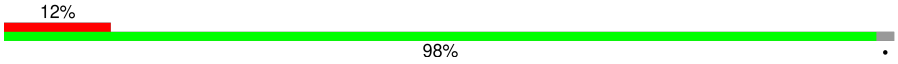
Chain Y:

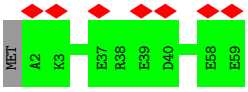




• Molecule 31: 50S ribosomal protein L30

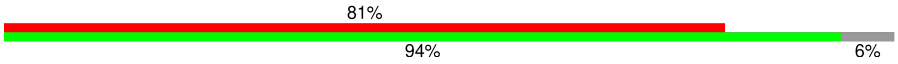
Chain Z:

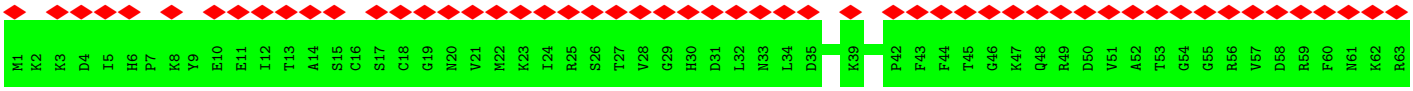


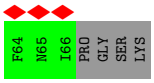


• Molecule 32: 50S ribosomal protein L31

Chain a:

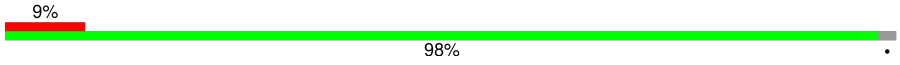


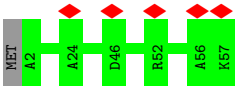




• Molecule 33: 50S ribosomal protein L32

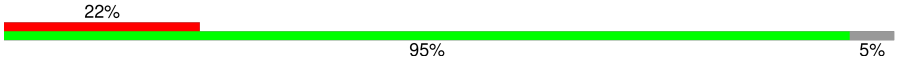
Chain b:

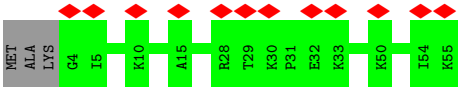




• Molecule 34: 50S ribosomal protein L33

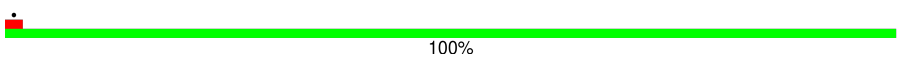
Chain c:





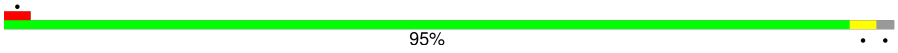
• Molecule 35: 50S ribosomal protein L34

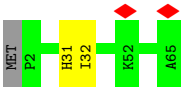
Chain d:



• Molecule 36: 50S ribosomal protein L35

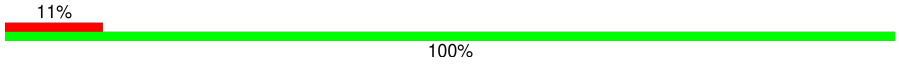
Chain e:

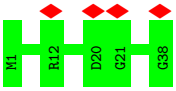




• Molecule 37: 50S ribosomal protein L36

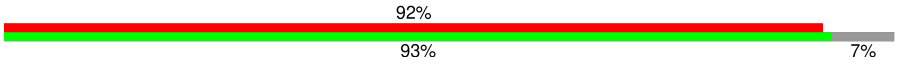
Chain f:

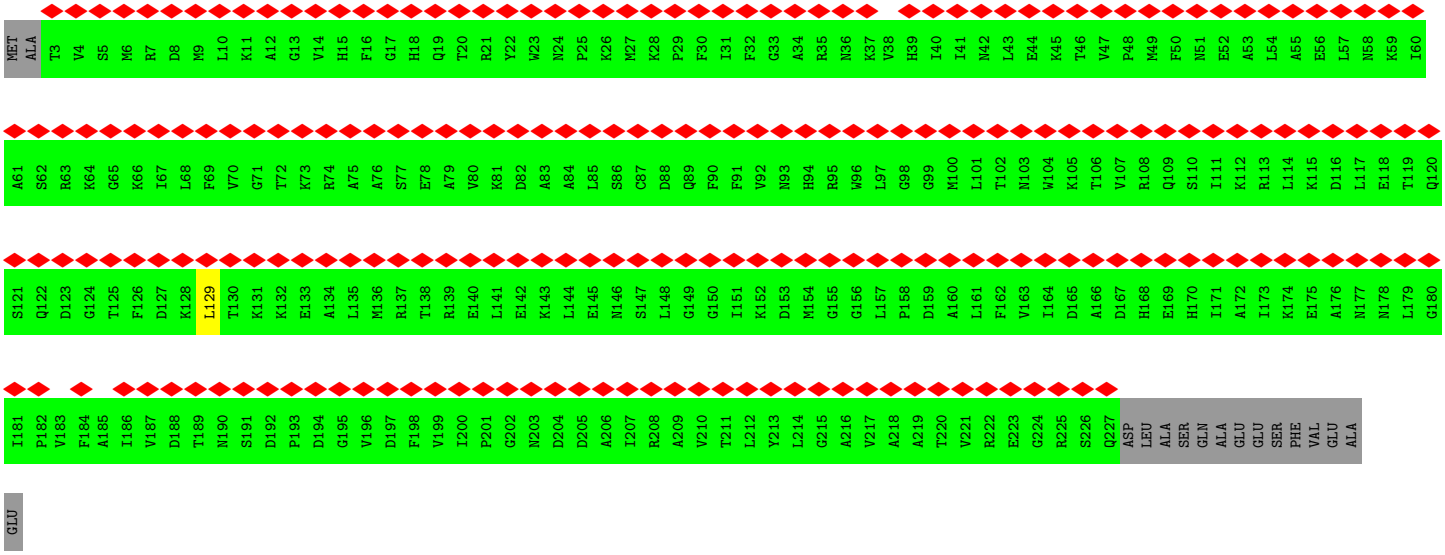




• Molecule 38: 30S ribosomal protein S2

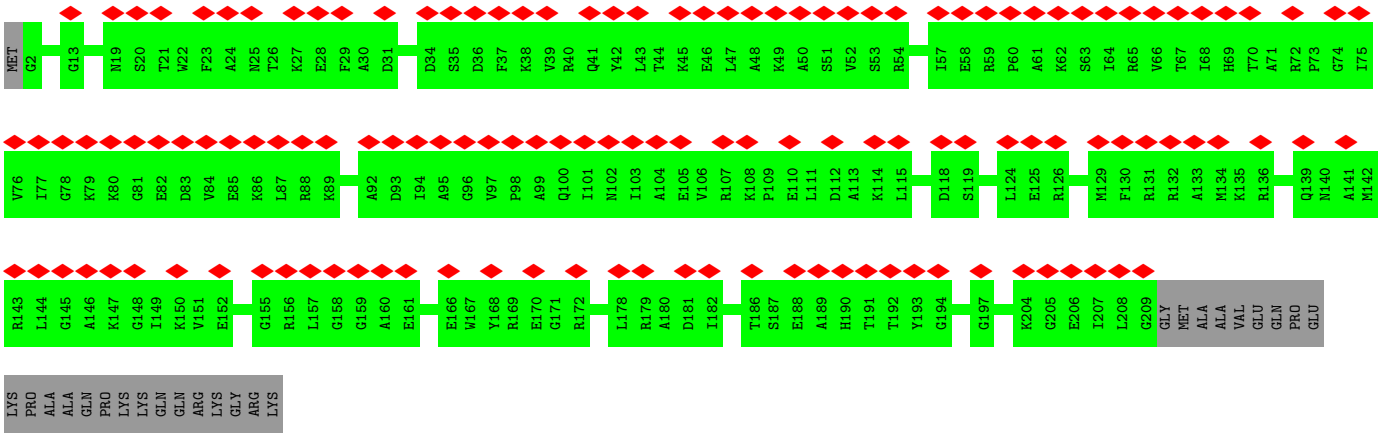
Chain g:





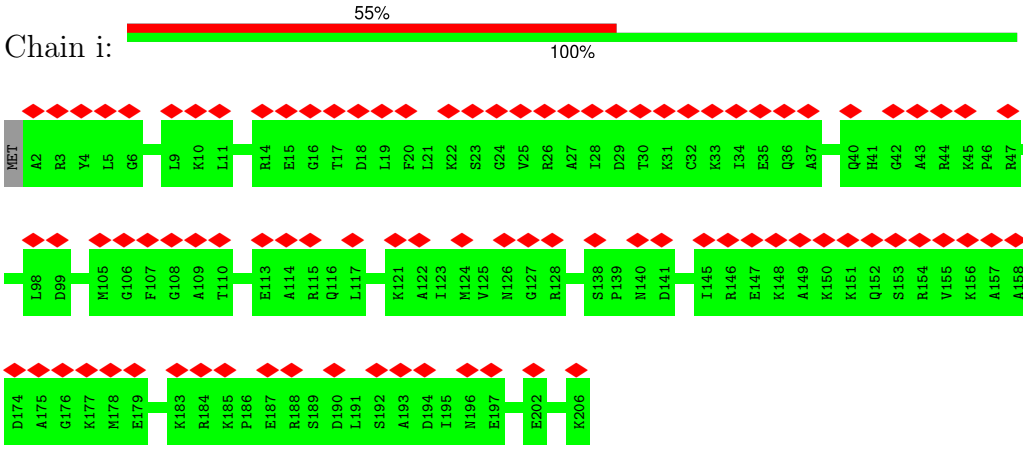
• Molecule 39: 30S ribosomal protein S3

Chain h:



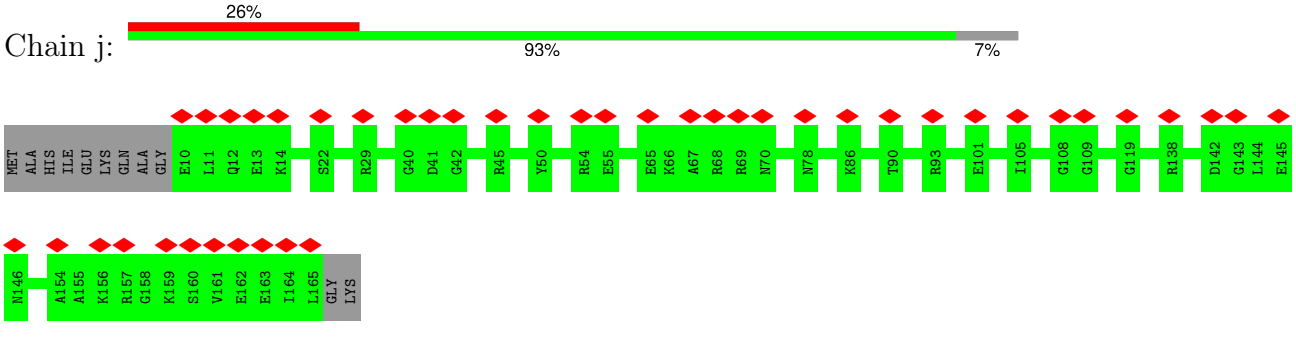
• Molecule 40: 30S ribosomal protein S4

Chain i:



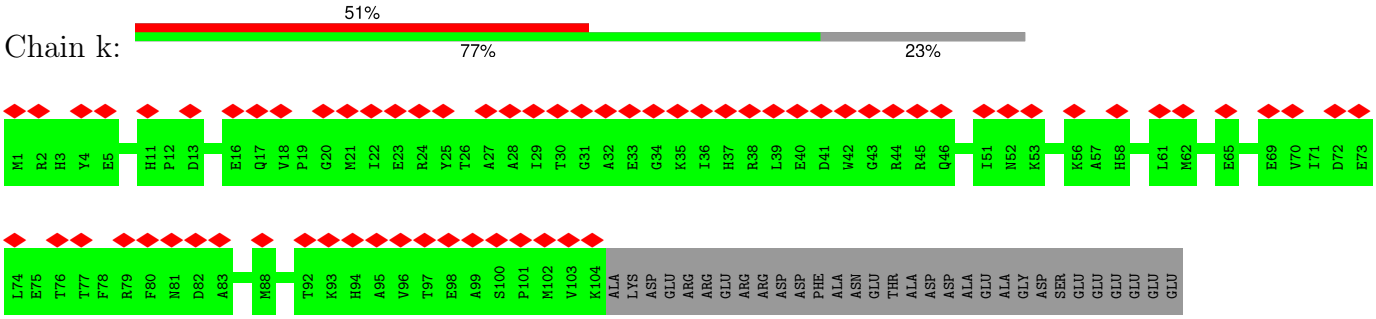
• Molecule 41: Small ribosomal subunit protein uS5

Chain j:



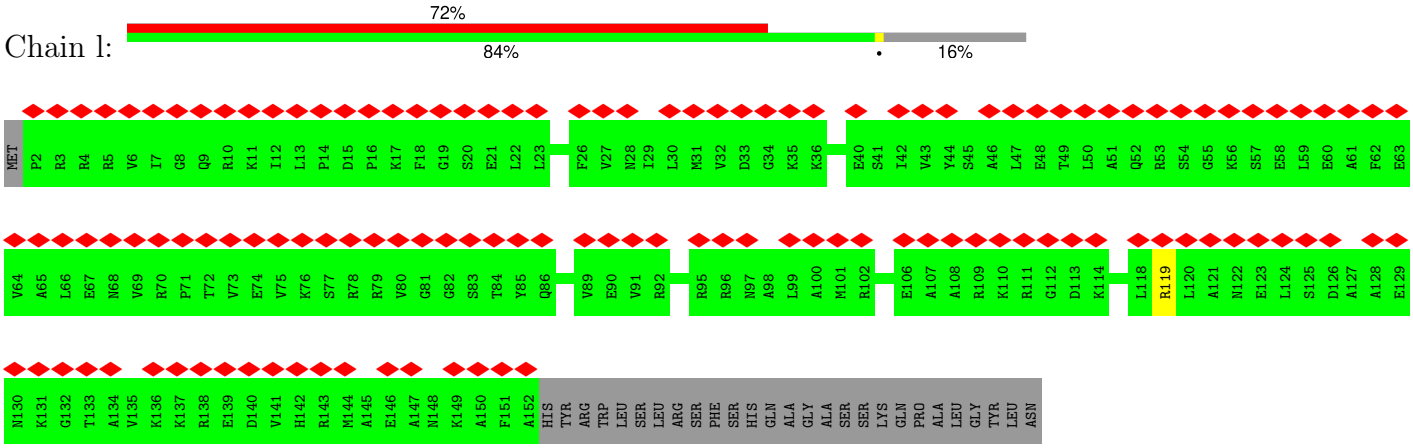
• Molecule 42: 30S ribosomal protein S6

Chain k:



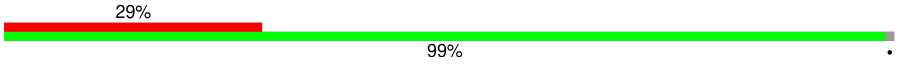
• Molecule 43: 30S ribosomal protein S7

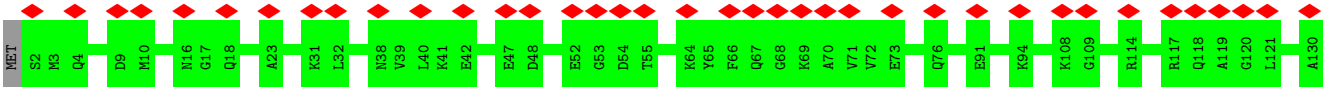
Chain l:



• Molecule 44: Small ribosomal subunit protein uS8

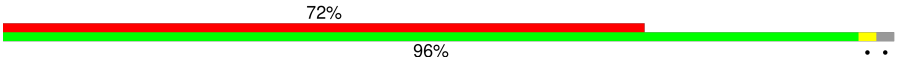
Chain m:

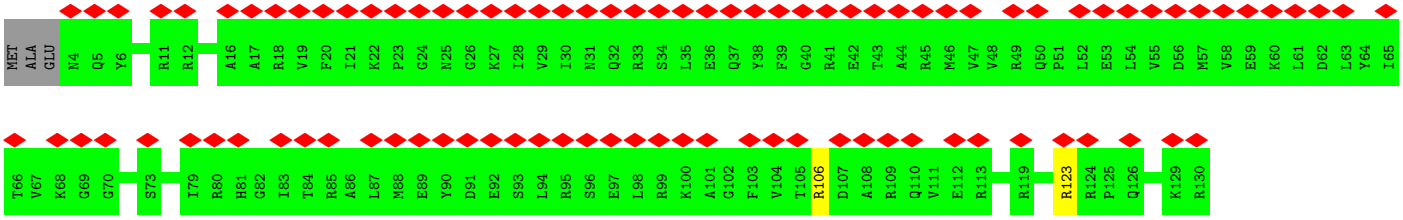




• Molecule 45: Small ribosomal subunit protein uS9

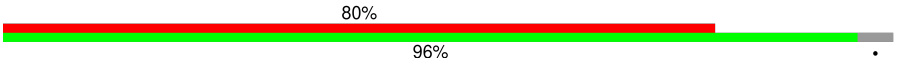
Chain n:





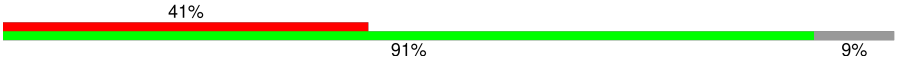
• Molecule 46: Small ribosomal subunit protein uS10

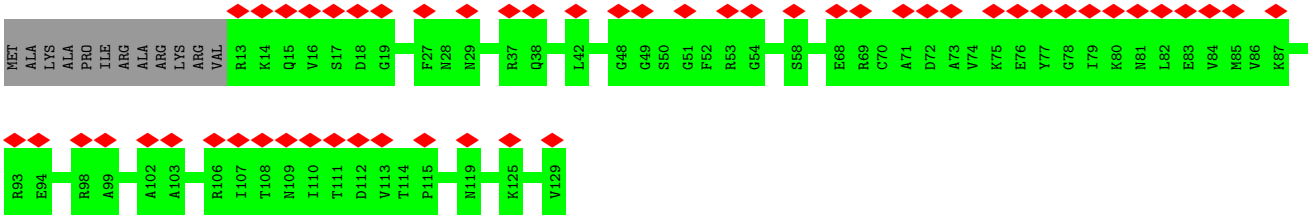
Chain o:



• Molecule 47: 30S ribosomal protein S11

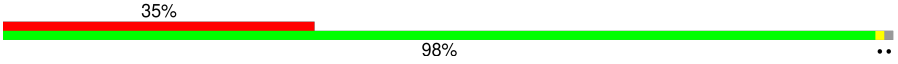
Chain p:

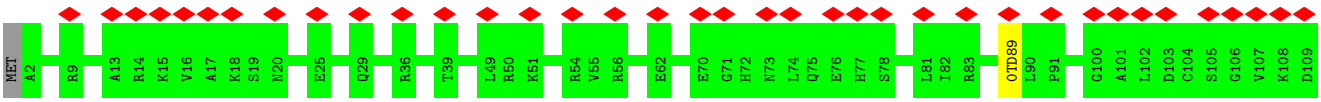


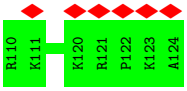


• Molecule 48: Small ribosomal subunit protein uS12

Chain q:

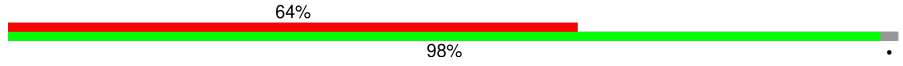


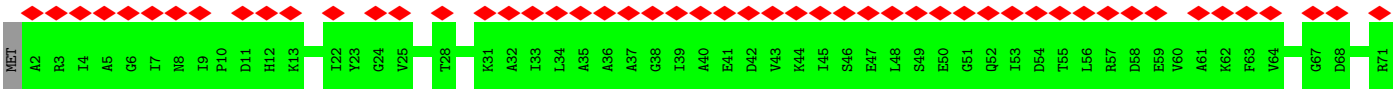


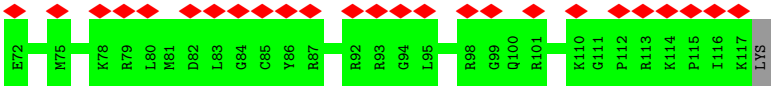


• Molecule 49: 30S ribosomal protein S13

Chain r:

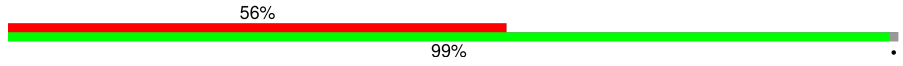


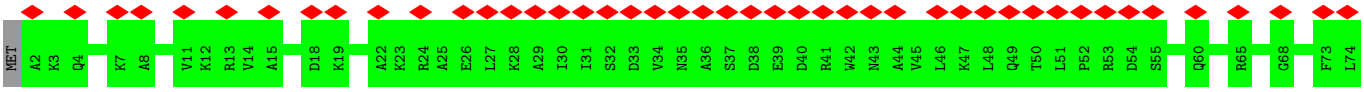


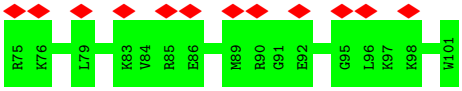


• Molecule 50: Small ribosomal subunit protein uS14

Chain s:

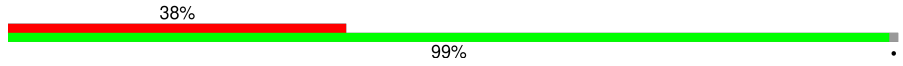


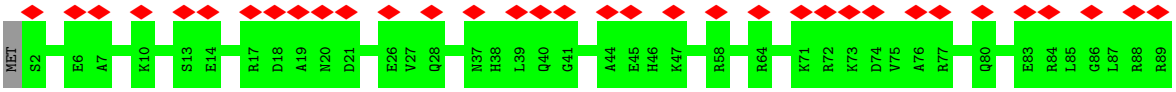




• Molecule 51: Small ribosomal subunit protein uS15

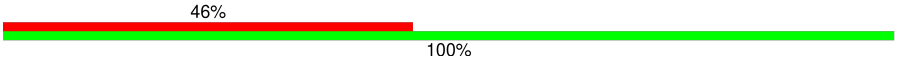
Chain t:

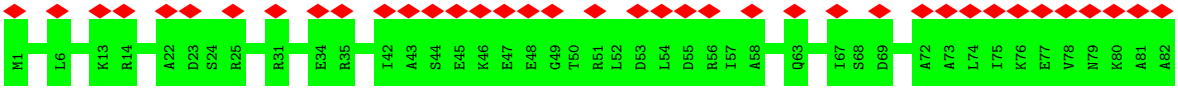




• Molecule 52: 30S ribosomal protein S16

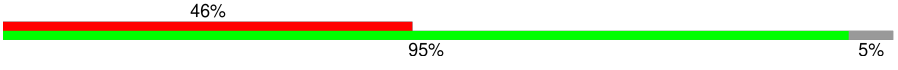
Chain u:

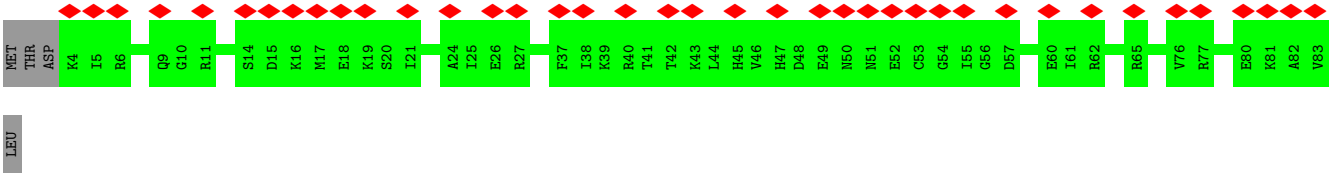




• Molecule 53: Small ribosomal subunit protein uS17

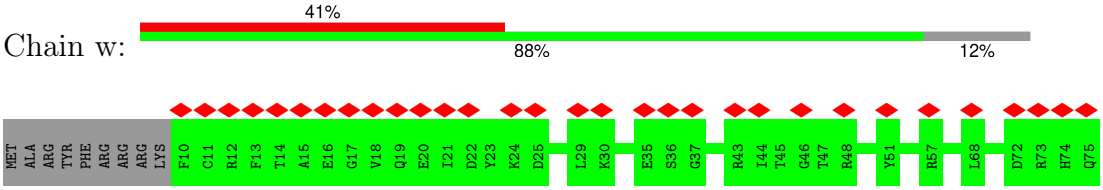
Chain v:





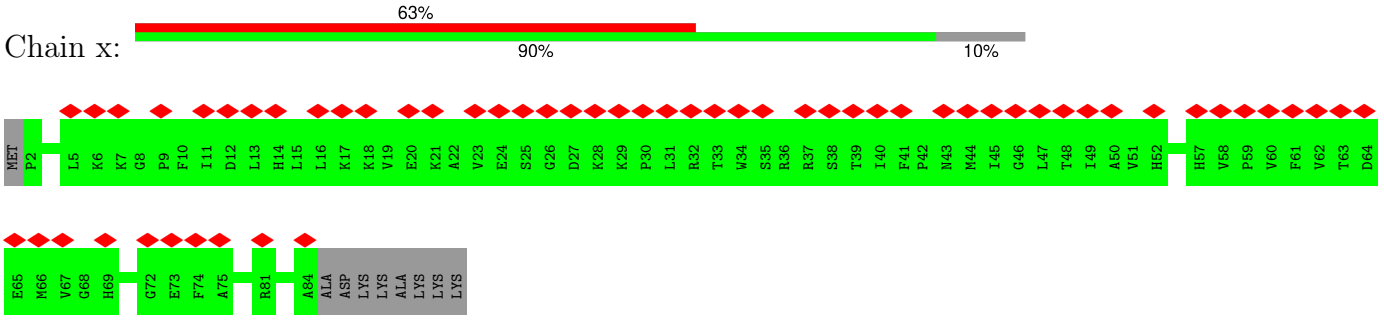
• Molecule 54: 30S ribosomal protein S18

Chain w:



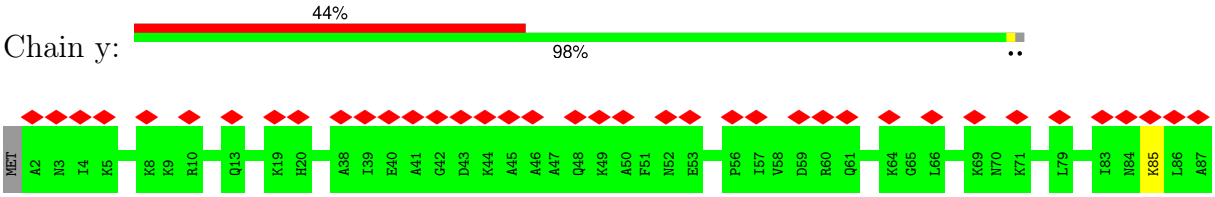
• Molecule 55: Small ribosomal subunit protein uS19

Chain x:



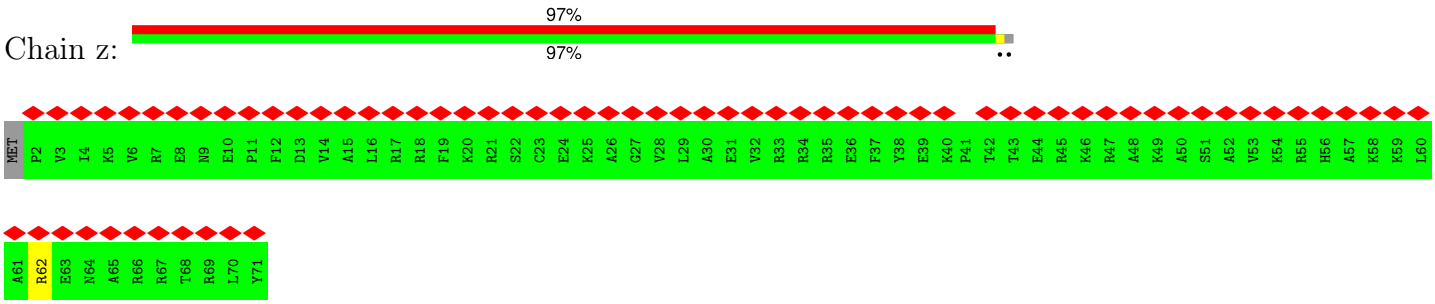
• Molecule 56: 30S ribosomal protein S20

Chain y:



• Molecule 57: 30S ribosomal protein S21

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104212	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.049	Depositor
Minimum map value	-0.537	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.456	Depositor
Map size (Å)	403.19998, 403.19998, 403.19998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 5MC, MA6, OMC, 2MG, 2MA, 0TD, UR3, 6MZ, 3TD, OMG, PSU, 4OC, 5MU, G7M, MG, ZN, 1MG

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	1	1.04	0/69285	0.90	26/108083 (0.0%)
2	2	0.90	0/36590	0.90	20/57074 (0.0%)
3	4	0.83	0/2872	0.90	0/4478
4	5	0.71	0/1835	0.88	0/2859
4	6	0.28	0/1832	0.84	0/2855
5	7	0.85	0/147	0.73	0/227
6	A	0.37	0/1869	0.57	0/2515
7	B	0.58	0/2121	0.58	0/2852
8	C	0.55	0/1586	0.58	0/2134
9	D	0.49	0/1571	0.57	0/2113
10	E	0.45	0/1434	0.58	0/1926
11	F	0.42	0/1333	0.56	0/1805
12	G	0.31	0/1122	0.54	0/1515
13	H	0.26	0/993	0.55	1/1340 (0.1%)
14	I	0.26	0/998	0.48	0/1348
15	J	0.54	0/1152	0.56	0/1551
16	K	0.51	0/955	0.56	0/1279
17	L	0.49	0/1062	0.58	0/1413
18	M	0.54	1/1093 (0.1%)	0.56	0/1460
19	N	0.52	0/964	0.59	0/1289
20	O	0.45	0/902	0.52	0/1209
21	P	0.53	0/929	0.55	0/1242
22	Q	0.61	0/960	0.55	0/1278
23	R	0.54	0/829	0.62	0/1107
24	S	0.49	0/864	0.54	0/1156
25	T	0.46	0/752	0.52	0/1005
26	U	0.46	0/796	0.53	1/1062 (0.1%)
27	V	0.45	0/766	0.55	0/1025
28	W	0.54	0/589	0.52	0/779
29	X	0.56	1/635 (0.2%)	0.57	0/848
30	Y	0.39	0/502	0.55	0/667

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	Z	0.46	0/452	0.63	0/605
32	a	0.36	0/531	0.52	0/709
33	b	0.49	0/450	0.56	0/599
34	c	0.44	0/433	0.52	0/576
35	d	0.49	0/380	0.50	0/498
36	e	0.52	0/513	0.59	0/676
37	f	0.48	0/303	0.55	0/397
38	g	0.30	0/1791	0.54	1/2413 (0.0%)
39	h	0.43	0/1663	0.55	0/2241
40	i	0.45	0/1665	0.50	0/2227
41	j	0.48	0/1165	0.58	0/1568
42	k	0.43	0/867	0.58	0/1171
43	l	0.37	0/1195	0.54	0/1602
44	m	0.47	0/989	0.59	0/1326
45	n	0.41	0/1034	0.54	0/1375
46	o	0.42	0/800	0.58	0/1082
47	p	0.42	0/893	0.52	0/1205
48	q	0.50	0/960	0.57	0/1286
49	r	0.38	0/909	0.52	0/1215
50	s	0.44	0/817	0.52	0/1088
51	t	0.44	0/722	0.55	0/964
52	u	0.49	0/659	0.55	0/884
53	v	0.43	0/657	0.59	0/881
54	w	0.45	0/553	0.55	0/743
55	x	0.40	0/680	0.54	0/915
56	y	0.42	0/675	0.49	0/895
57	z	0.29	0/597	0.44	0/792
All	All	0.85	2/161691 (0.0%)	0.82	49/241427 (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
1	1	3	0
6	A	0	1
12	G	0	1
36	e	0	1
All	All	3	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	29	PHE	C-N	-5.19	1.22	1.34
18	M	96	ILE	C-N	-5.05	1.22	1.34

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	1109	C	O4'-C1'-N1	-8.69	101.25	108.20
2	2	1132	C	C2-N1-C1'	8.39	128.03	118.80
2	2	328	C	C2-N1-C1'	8.33	127.96	118.80
2	2	328	C	N1-C2-O2	8.01	123.70	118.90
2	2	20	U	C2-N3-C4	-7.88	122.27	127.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	2069	G7M	C2',C3',C4'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	106	GLN	Peptide
12	G	9	VAL	Peptide
36	e	31	HIS	Peptide

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
6	A	227/231 (98%)	201 (88%)	24 (11%)	2 (1%)	14 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	B	269/273 (98%)	252 (94%)	17 (6%)	0	100	100
8	C	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
9	D	199/201 (99%)	187 (94%)	12 (6%)	0	100	100
10	E	175/179 (98%)	164 (94%)	10 (6%)	1 (1%)	22	48
11	F	173/177 (98%)	160 (92%)	13 (8%)	0	100	100
12	G	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
13	H	128/165 (78%)	111 (87%)	17 (13%)	0	100	100
14	I	133/142 (94%)	122 (92%)	11 (8%)	0	100	100
15	J	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
16	K	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
17	L	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
18	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
19	N	117/127 (92%)	113 (97%)	4 (3%)	0	100	100
20	O	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
21	P	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
22	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
23	R	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
24	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
25	T	92/100 (92%)	89 (97%)	3 (3%)	0	100	100
26	U	101/104 (97%)	92 (91%)	9 (9%)	0	100	100
27	V	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
28	W	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
29	X	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
30	Y	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
31	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
32	a	64/70 (91%)	59 (92%)	5 (8%)	0	100	100
33	b	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
34	c	50/55 (91%)	47 (94%)	3 (6%)	0	100	100
35	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
36	e	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	8	24
37	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	g	223/241 (92%)	207 (93%)	16 (7%)	0	100	100
39	h	206/233 (88%)	196 (95%)	10 (5%)	0	100	100
40	i	203/206 (98%)	197 (97%)	6 (3%)	0	100	100
41	j	154/167 (92%)	143 (93%)	11 (7%)	0	100	100
42	k	102/135 (76%)	97 (95%)	5 (5%)	0	100	100
43	l	149/179 (83%)	141 (95%)	8 (5%)	0	100	100
44	m	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
45	n	125/130 (96%)	114 (91%)	11 (9%)	0	100	100
46	o	97/103 (94%)	89 (92%)	8 (8%)	0	100	100
47	p	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
48	q	120/124 (97%)	110 (92%)	10 (8%)	0	100	100
49	r	114/118 (97%)	106 (93%)	8 (7%)	0	100	100
50	s	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
51	t	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
52	u	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
53	v	78/84 (93%)	70 (90%)	8 (10%)	0	100	100
54	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
55	x	81/92 (88%)	77 (95%)	4 (5%)	0	100	100
56	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
57	z	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	6096/6451 (94%)	5738 (94%)	354 (6%)	4 (0%)	50	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	212	LYS
6	A	88	HIS
10	E	123	ASP
36	e	32	ILE

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
6	A	199/201 (99%)	199 (100%)	0	100 100
7	B	216/218 (99%)	216 (100%)	0	100 100
8	C	164/164 (100%)	164 (100%)	0	100 100
9	D	165/165 (100%)	164 (99%)	1 (1%)	84 94
10	E	148/150 (99%)	148 (100%)	0	100 100
11	F	136/138 (99%)	136 (100%)	0	100 100
12	G	114/114 (100%)	114 (100%)	0	100 100
13	H	99/123 (80%)	99 (100%)	0	100 100
14	I	104/110 (94%)	104 (100%)	0	100 100
15	J	116/116 (100%)	116 (100%)	0	100 100
16	K	104/104 (100%)	104 (100%)	0	100 100
17	L	103/103 (100%)	103 (100%)	0	100 100
18	M	109/109 (100%)	109 (100%)	0	100 100
19	N	99/103 (96%)	99 (100%)	0	100 100
20	O	86/87 (99%)	86 (100%)	0	100 100
21	P	99/100 (99%)	99 (100%)	0	100 100
22	Q	89/90 (99%)	89 (100%)	0	100 100
23	R	84/84 (100%)	84 (100%)	0	100 100
24	S	93/93 (100%)	92 (99%)	1 (1%)	70 88
25	T	81/84 (96%)	81 (100%)	0	100 100
26	U	84/85 (99%)	83 (99%)	1 (1%)	67 87
27	V	78/78 (100%)	78 (100%)	0	100 100
28	W	58/63 (92%)	57 (98%)	1 (2%)	56 81
29	X	67/68 (98%)	67 (100%)	0	100 100
30	Y	54/55 (98%)	54 (100%)	0	100 100
31	Z	48/49 (98%)	48 (100%)	0	100 100
32	a	59/62 (95%)	59 (100%)	0	100 100
33	b	47/48 (98%)	47 (100%)	0	100 100
34	c	47/49 (96%)	47 (100%)	0	100 100
35	d	38/38 (100%)	38 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	e	51/52 (98%)	51 (100%)	0	100 100
37	f	34/34 (100%)	34 (100%)	0	100 100
38	g	187/199 (94%)	187 (100%)	0	100 100
39	h	171/190 (90%)	171 (100%)	0	100 100
40	i	172/173 (99%)	172 (100%)	0	100 100
41	j	119/126 (94%)	119 (100%)	0	100 100
42	k	91/116 (78%)	91 (100%)	0	100 100
43	l	124/147 (84%)	123 (99%)	1 (1%)	79 92
44	m	104/105 (99%)	104 (100%)	0	100 100
45	n	105/107 (98%)	103 (98%)	2 (2%)	52 79
46	o	86/90 (96%)	86 (100%)	0	100 100
47	p	90/99 (91%)	90 (100%)	0	100 100
48	q	102/103 (99%)	102 (100%)	0	100 100
49	r	94/96 (98%)	94 (100%)	0	100 100
50	s	83/84 (99%)	83 (100%)	0	100 100
51	t	76/77 (99%)	76 (100%)	0	100 100
52	u	65/65 (100%)	65 (100%)	0	100 100
53	v	74/78 (95%)	74 (100%)	0	100 100
54	w	57/65 (88%)	57 (100%)	0	100 100
55	x	72/79 (91%)	72 (100%)	0	100 100
56	y	65/66 (98%)	64 (98%)	1 (2%)	60 84
57	z	60/61 (98%)	59 (98%)	1 (2%)	56 81
All	All	5070/5263 (96%)	5061 (100%)	9 (0%)	91 97

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

Mol	Chain	Res	Type
56	y	85	LYS
57	z	62	ARG
28	W	14	ARG
43	l	119	ARG
45	n	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
38	g	39	HIS
48	q	5	ASN
49	r	100	GLN
45	n	5	GLN
18	M	45	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2896/2903 (99%)	529 (18%)	13 (0%)
2	2	1529/1534 (99%)	279 (18%)	6 (0%)
3	4	119/120 (99%)	21 (17%)	0
4	5	76/77 (98%)	18 (23%)	1 (1%)
4	6	76/77 (98%)	17 (22%)	1 (1%)
5	7	5/25 (20%)	1 (20%)	0
All	All	4701/4736 (99%)	865 (18%)	21 (0%)

5 of 865 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	13	A
1	1	15	G
1	1	23	G
1	1	34	U

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1004	A
2	2	1167	A
4	6	18	U
2	2	1493	A
2	2	1145	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	1MG	1	745	1	19,26,27	0.76	0	18,39,42	1.23	2 (11%)
1	2MG	1	1835	1	18,26,27	0.96	1 (5%)	16,38,41	1.56	6 (37%)
2	PSU	2	516	58,2	18,21,22	1.06	2 (11%)	21,30,33	1.77	4 (19%)
2	5MC	2	1407	2	19,22,23	1.31	3 (15%)	26,32,35	1.20	2 (7%)
1	PSU	1	2457	1	18,21,22	1.13	3 (16%)	21,30,33	2.25	6 (28%)
2	5MC	2	967	2	19,22,23	1.36	3 (15%)	26,32,35	1.09	2 (7%)
1	2MA	1	2503	58,1	18,25,26	0.72	0	20,37,40	2.00	3 (15%)
2	G7M	2	527	2	20,26,27	2.44	4 (20%)	16,39,42	0.98	1 (6%)
1	OMG	1	2251	4,1	19,26,27	1.01	1 (5%)	21,38,41	1.10	3 (14%)
2	4OC	2	1402	2	20,23,24	0.83	1 (5%)	25,32,35	0.92	1 (4%)
1	3TD	1	1915	58,1	19,22,23	2.93	4 (21%)	23,32,35	7.31	6 (26%)
1	5MU	1	747	1	19,22,23	1.40	4 (21%)	27,32,35	2.31	6 (22%)
1	PSU	1	2504	1	18,21,22	1.12	2 (11%)	21,30,33	1.86	4 (19%)
1	PSU	1	955	1	18,21,22	1.13	2 (11%)	21,30,33	2.18	4 (19%)
2	MA6	2	1519	2	19,26,27	0.79	0	18,38,41	2.35	7 (38%)
1	5MU	1	1939	1	19,22,23	1.47	4 (21%)	27,32,35	2.44	6 (22%)
1	5MC	1	1962	1	19,22,23	1.25	2 (10%)	26,32,35	1.18	2 (7%)
1	PSU	1	1911	1	18,21,22	1.11	3 (16%)	21,30,33	2.04	5 (23%)
1	OMC	1	2498	58,1	19,22,23	0.96	2 (10%)	25,31,34	1.01	1 (4%)
1	2MG	1	2445	1	18,26,27	1.04	1 (5%)	16,38,41	1.49	4 (25%)
1	PSU	1	2605	1	18,21,22	1.04	2 (11%)	21,30,33	1.89	3 (14%)
1	6MZ	1	2030	58,1	17,25,26	0.84	0	15,36,39	2.58	4 (26%)
1	G7M	1	2069	1	20,26,27	1.15	2 (10%)	16,39,42	1.34	1 (6%)
1	OMU	1	2552	1	19,22,23	1.35	4 (21%)	25,31,34	1.98	5 (20%)
2	2MG	2	966	2	18,26,27	1.00	1 (5%)	16,38,41	1.46	5 (31%)
48	0TD	q	89	48	8,9,10	2.25	2 (25%)	6,11,13	2.10	2 (33%)
1	PSU	1	1917	1	18,21,22	1.03	2 (11%)	21,30,33	1.99	4 (19%)
2	2MG	2	1207	2	18,26,27	0.99	1 (5%)	16,38,41	1.44	5 (31%)
1	6MZ	1	1618	1	17,25,26	0.87	0	15,36,39	2.86	4 (26%)
2	MA6	2	1518	2	19,26,27	0.85	0	18,38,41	2.33	6 (33%)
2	UR3	2	1498	2	19,22,23	0.97	2 (10%)	26,32,35	1.73	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	2MG	2	1516	2	18,26,27	1.02	1 (5%)	16,38,41	1.55	5 (31%)
1	PSU	1	2580	58,1	18,21,22	1.18	3 (16%)	21,30,33	1.89	5 (23%)
1	PSU	1	746	58,1	18,21,22	1.13	3 (16%)	21,30,33	1.84	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	1MG	1	745	1	-	0/3/25/26	0/3/3/3
1	2MG	1	1835	1	-	2/5/27/28	0/3/3/3
2	PSU	2	516	58,2	-	4/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
1	PSU	1	2457	1	-	0/7/25/26	0/2/2/2
2	5MC	2	967	2	-	2/7/25/26	0/2/2/2
1	2MA	1	2503	58,1	-	2/3/25/26	0/3/3/3
2	G7M	2	527	2	-	2/3/25/26	0/3/3/3
1	OMG	1	2251	4,1	-	0/5/27/28	0/3/3/3
2	4OC	2	1402	2	-	0/9/29/30	0/2/2/2
1	3TD	1	1915	58,1	-	4/7/25/26	0/2/2/2
1	5MU	1	747	1	-	1/7/25/26	0/2/2/2
1	PSU	1	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	1	955	1	-	0/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	4/7/29/30	0/3/3/3
1	5MU	1	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	1	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	1	1911	1	-	2/7/25/26	0/2/2/2
1	OMC	1	2498	58,1	-	0/9/27/28	0/2/2/2
1	2MG	1	2445	1	-	2/5/27/28	0/3/3/3
1	PSU	1	2605	1	-	0/7/25/26	0/2/2/2
1	6MZ	1	2030	58,1	-	2/5/27/28	0/3/3/3
1	G7M	1	2069	1	3/3/5/5	2/3/25/26	0/3/3/3
1	OMU	1	2552	1	-	0/9/27/28	0/2/2/2
2	2MG	2	966	2	-	2/5/27/28	0/3/3/3
48	0TD	q	89	48	-	1/7/12/14	-
1	PSU	1	1917	1	-	0/7/25/26	0/2/2/2
2	2MG	2	1207	2	-	0/5/27/28	0/3/3/3
1	6MZ	1	1618	1	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MA6	2	1518	2	-	2/7/29/30	0/3/3/3
2	UR3	2	1498	2	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/5/27/28	0/3/3/3
1	PSU	1	2580	58,1	-	0/7/25/26	0/2/2/2
1	PSU	1	746	58,1	-	4/7/25/26	0/2/2/2

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1915	3TD	C6-C5	-9.13	1.25	1.35
2	2	527	G7M	C8-N9	6.91	1.45	1.33
2	2	527	G7M	C8-N7	6.50	1.45	1.33
1	1	1915	3TD	C6-N1	-6.50	1.25	1.36
48	q	89	0TD	CB-CA	-4.72	1.53	1.54

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1915	3TD	C5-C6-N1	25.17	157.09	122.14
1	1	1915	3TD	C6-C5-C4	-20.35	104.56	118.19
1	1	1915	3TD	C1'-C5-C4	8.45	130.44	117.61
1	1	1915	3TD	C6-N1-C2	-8.28	100.70	121.80
1	1	1618	6MZ	C9-N6-C6	-7.71	115.70	122.85

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	2069	G7M	C2'
1	1	2069	G7M	C3'
1	1	2069	G7M	C4'

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	967	5MC	C3'-C4'-C5'-O5'
2	2	1518	MA6	C5-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 441 ligands modelled in this entry, 441 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1914:C	O3'	1915:3TD	P	7.81
1	1	2314:A	O3'	2315:G	P	3.31

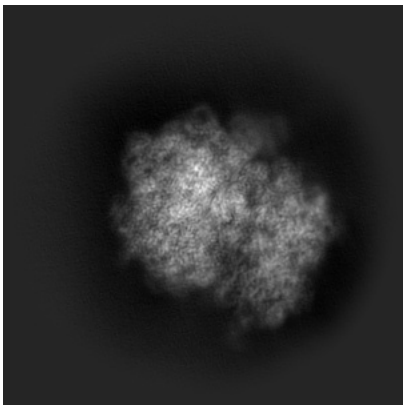
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-48513. These allow visual inspection of the internal detail of the map and identification of artifacts.

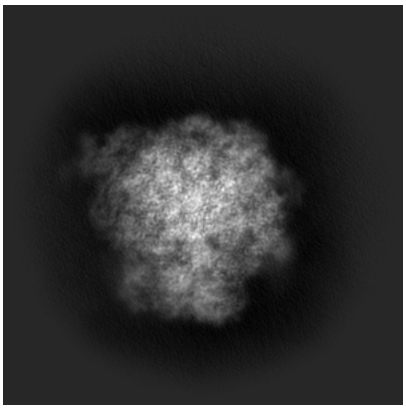
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

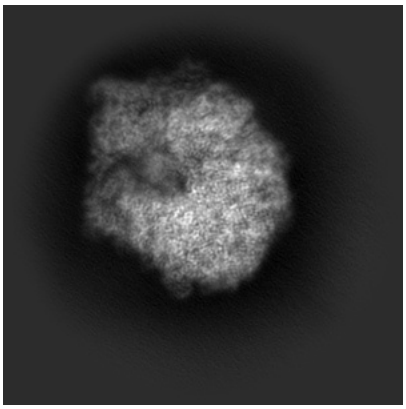
6.1.1 Primary map



X

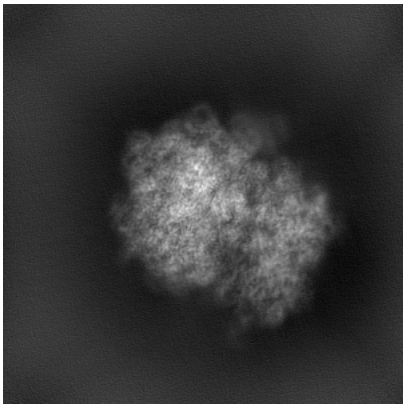


Y

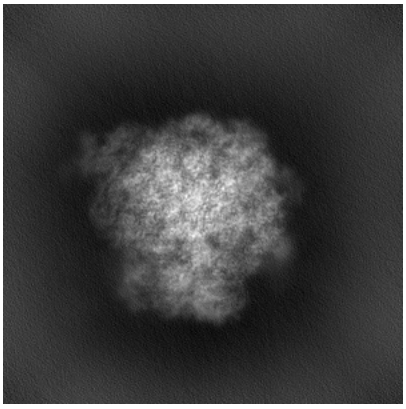


Z

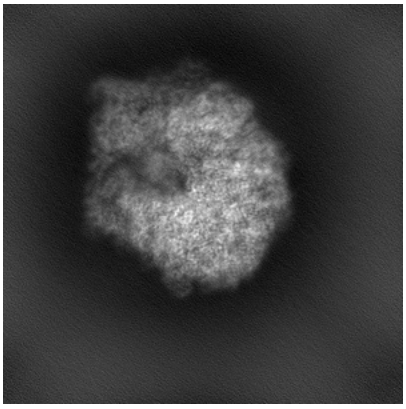
6.1.2 Raw map



X



Y

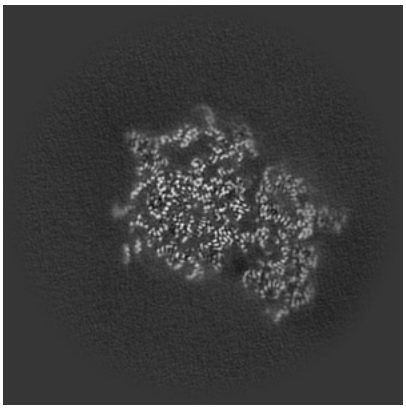


Z

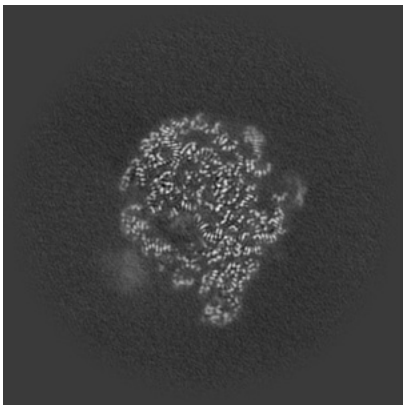
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

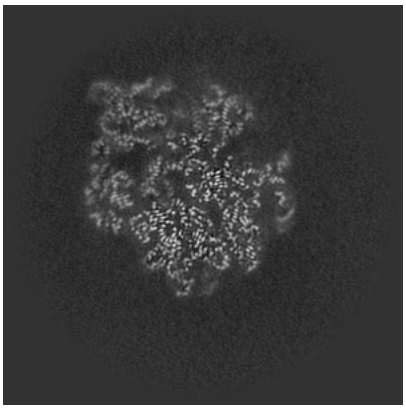
6.2.1 Primary map



X Index: 192

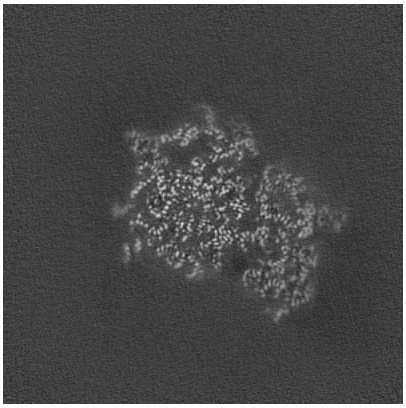


Y Index: 192

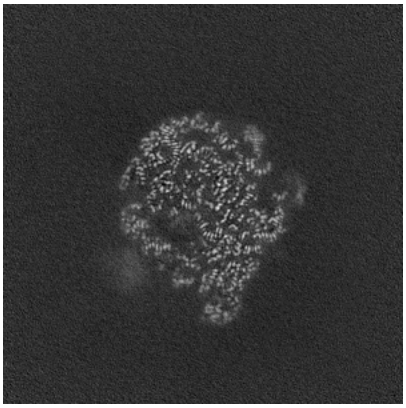


Z Index: 192

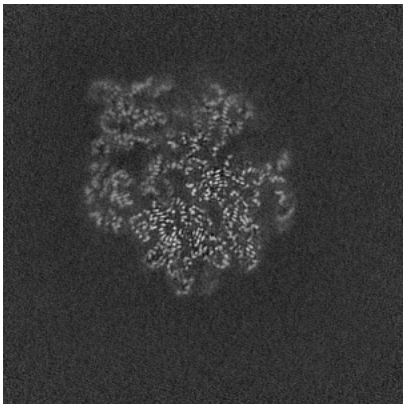
6.2.2 Raw map



X Index: 192



Y Index: 192

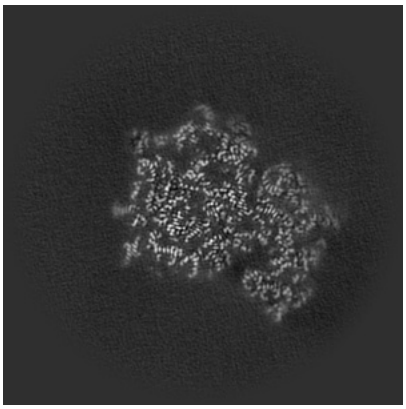


Z Index: 192

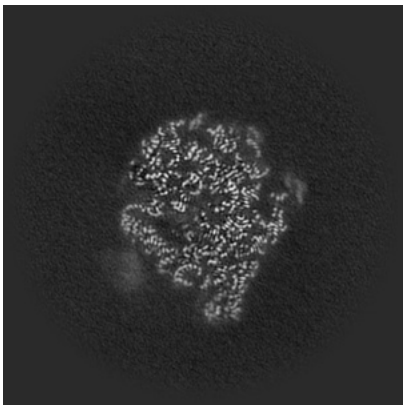
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

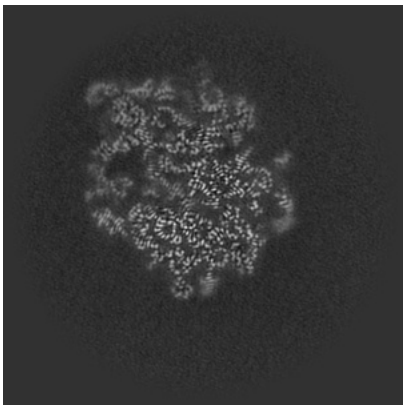
6.3.1 Primary map



X Index: 195

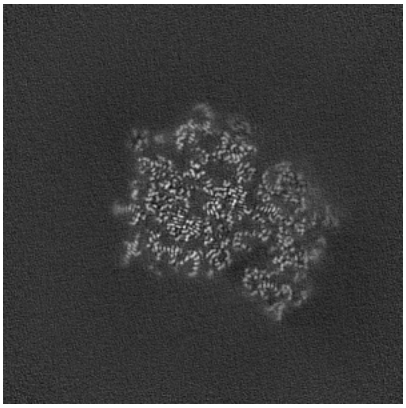


Y Index: 189

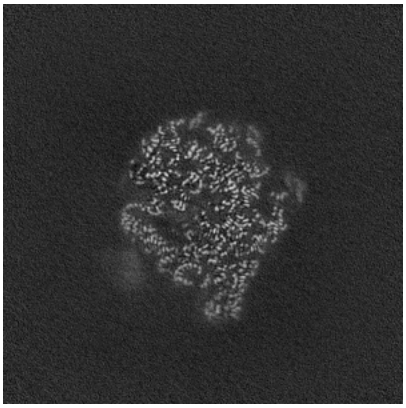


Z Index: 187

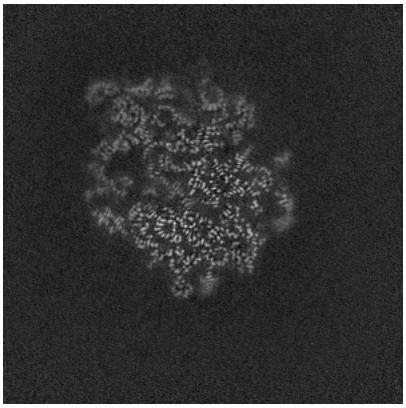
6.3.2 Raw map



X Index: 196



Y Index: 189

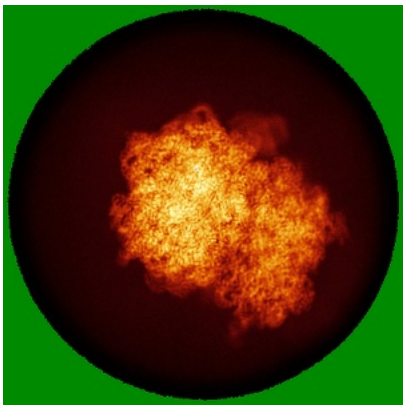


Z Index: 187

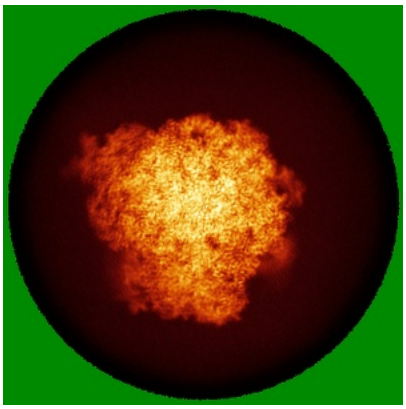
The images above show the largest variance slices of the map in three orthogonal directions.

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

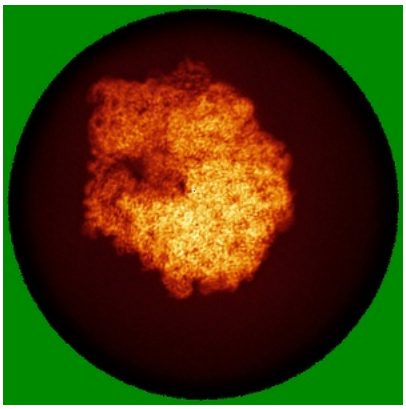
6.4.1 Primary map



X

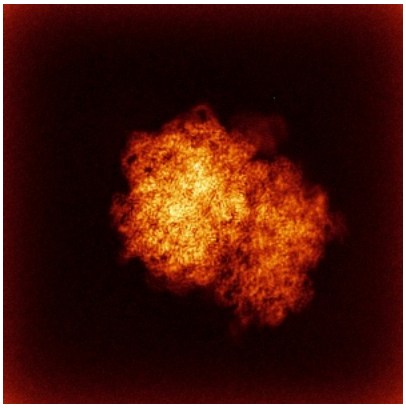


Y

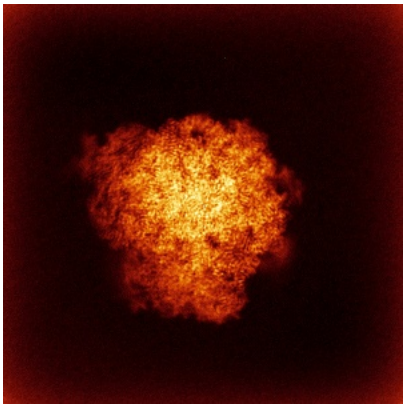


Z

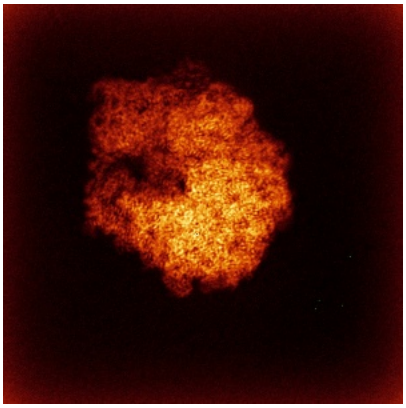
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.456. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

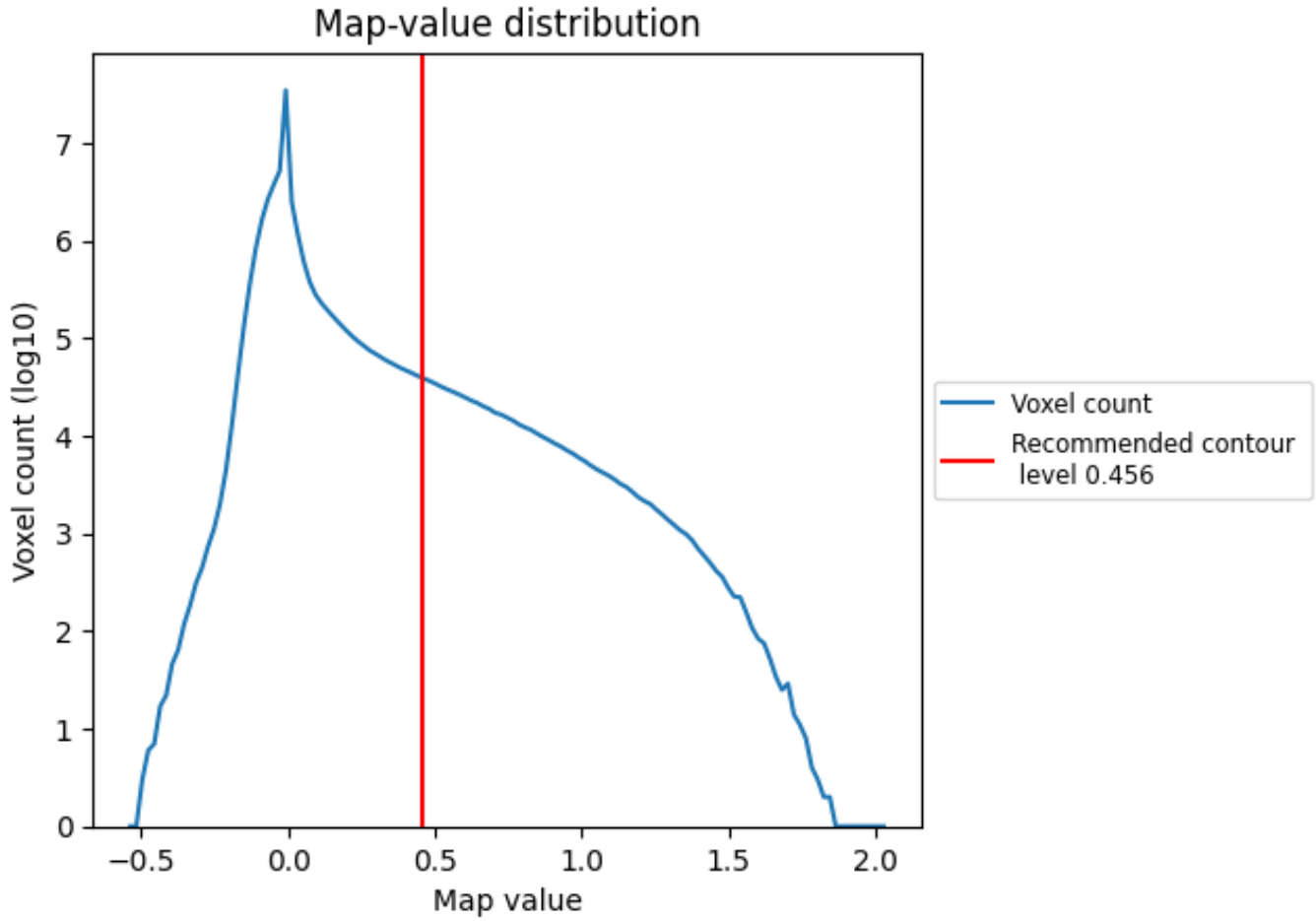
6.6 Mask visualisation (i)

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

7 Map analysis

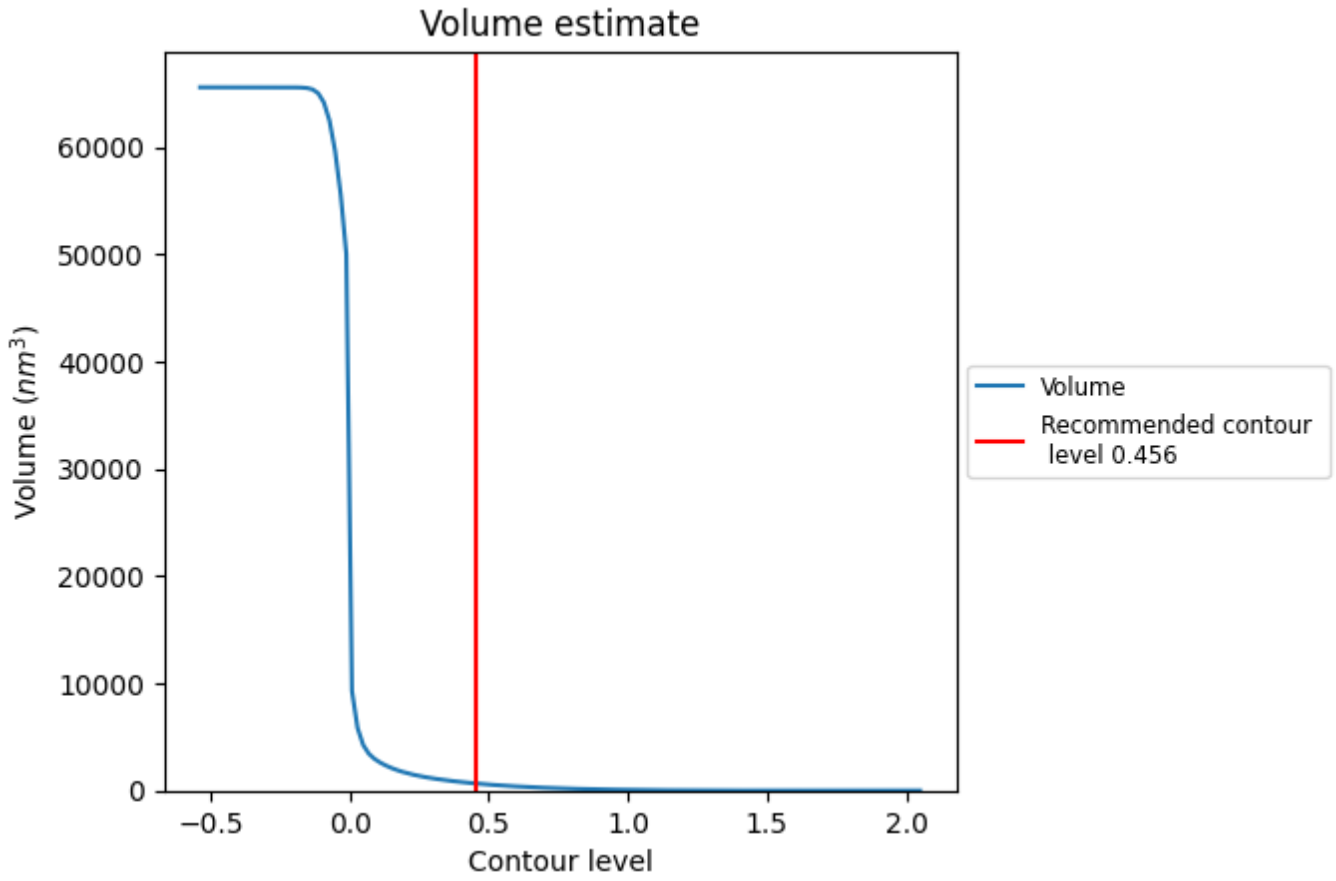
This section contains the results of statistical analysis of the map.

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.

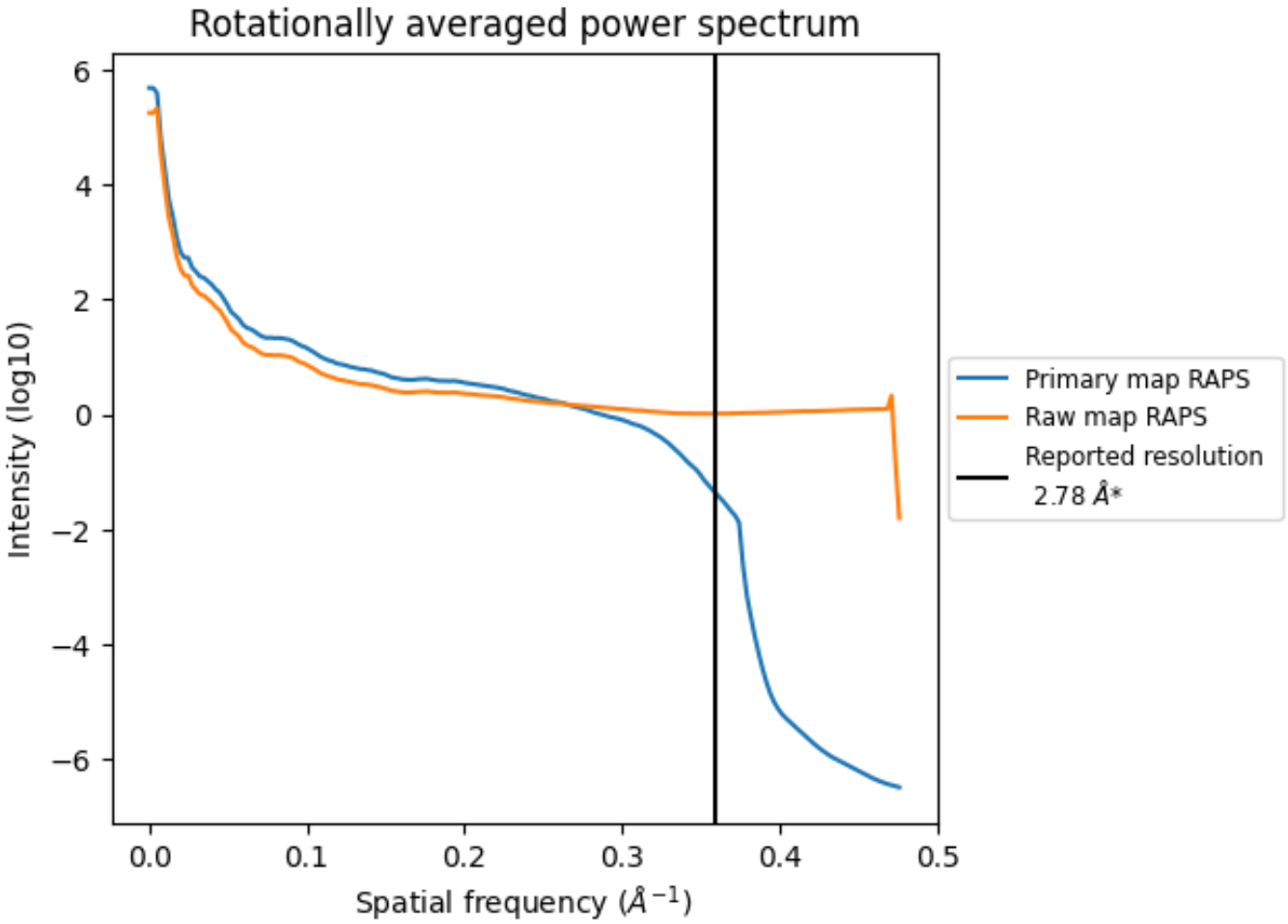
7.2 Volume estimate (i)



The volume at the recommended contour level is 654 nm^3; this corresponds to an approximate mass of 591 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)

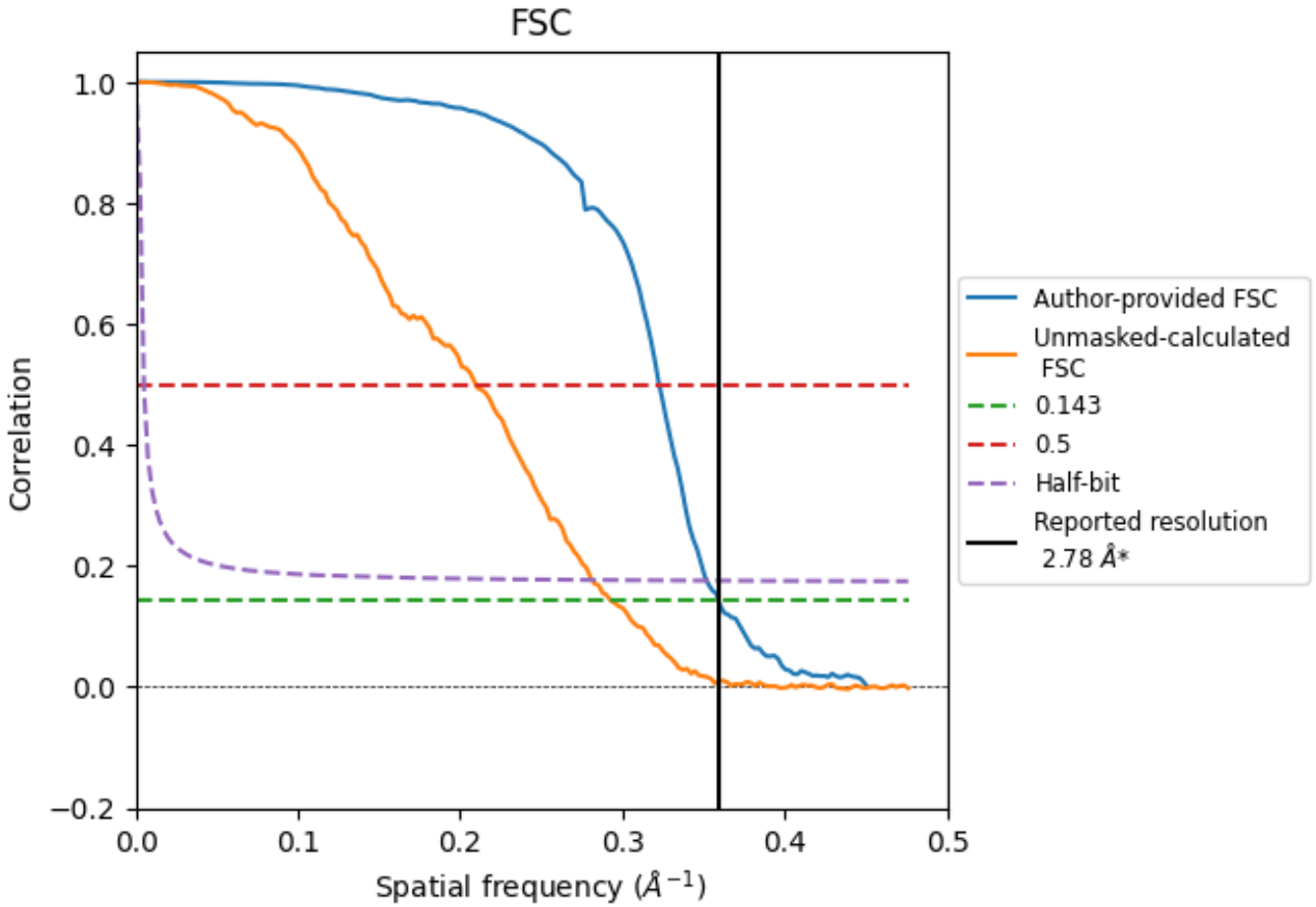


*Reported resolution corresponds to spatial frequency of 0.360 Å^{-1}

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 0.360 Å^{-1}

8.2 Resolution estimates (i)

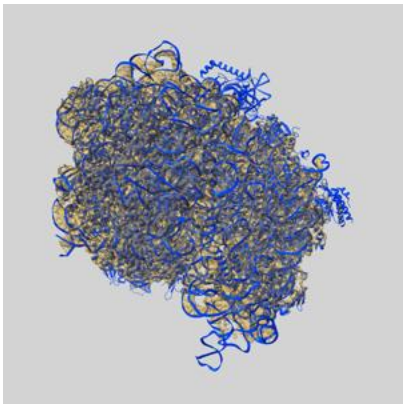
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	2.78	3.10	2.84
Unmasked-calculated*	3.42	4.77	3.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 2.78 by more than 10 %

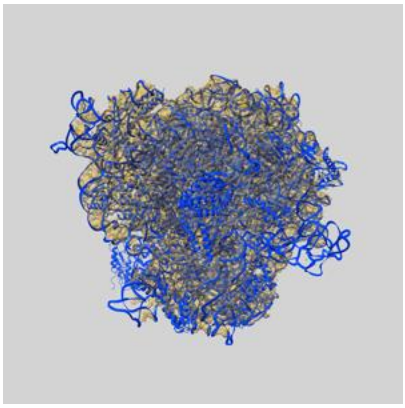
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48513 and PDB model 9MQ4. Per-residue inclusion information can be found in section 3 on page 16.

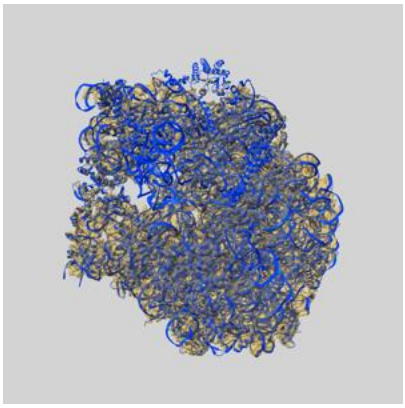
9.1 Map-model overlay



X



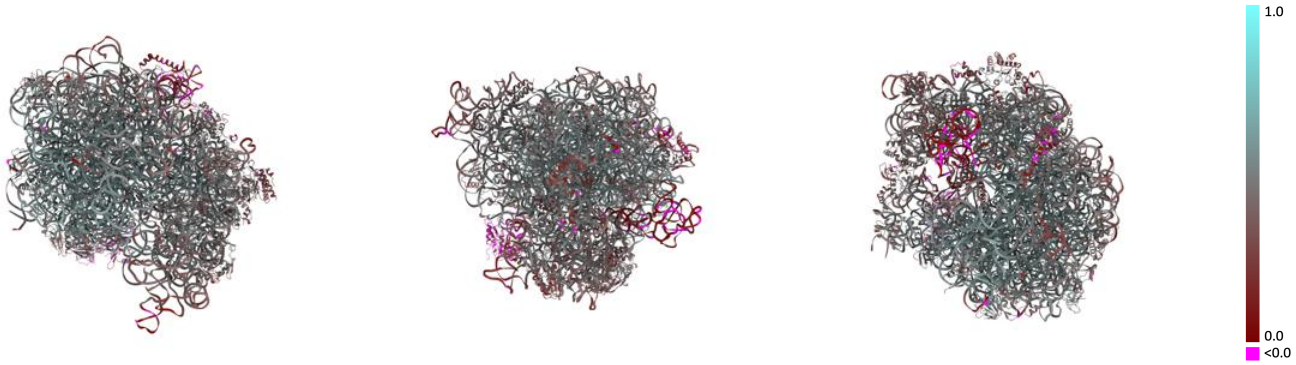
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.456 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

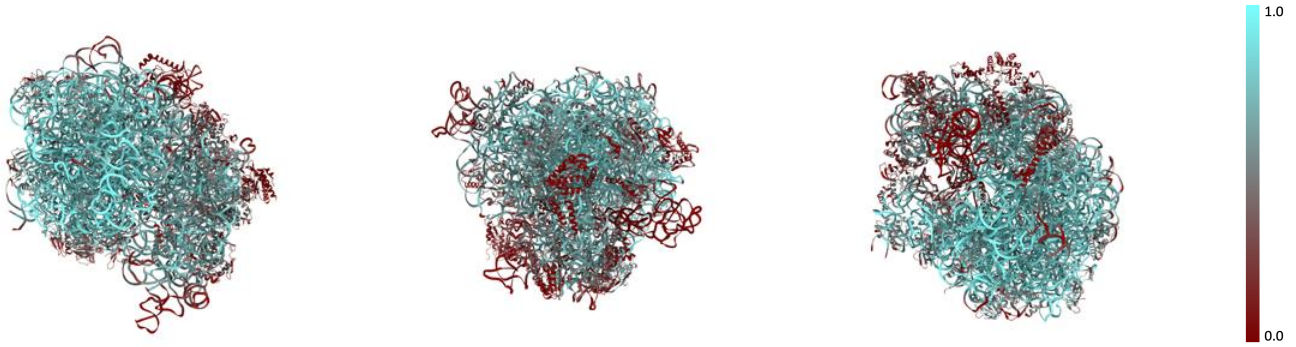
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

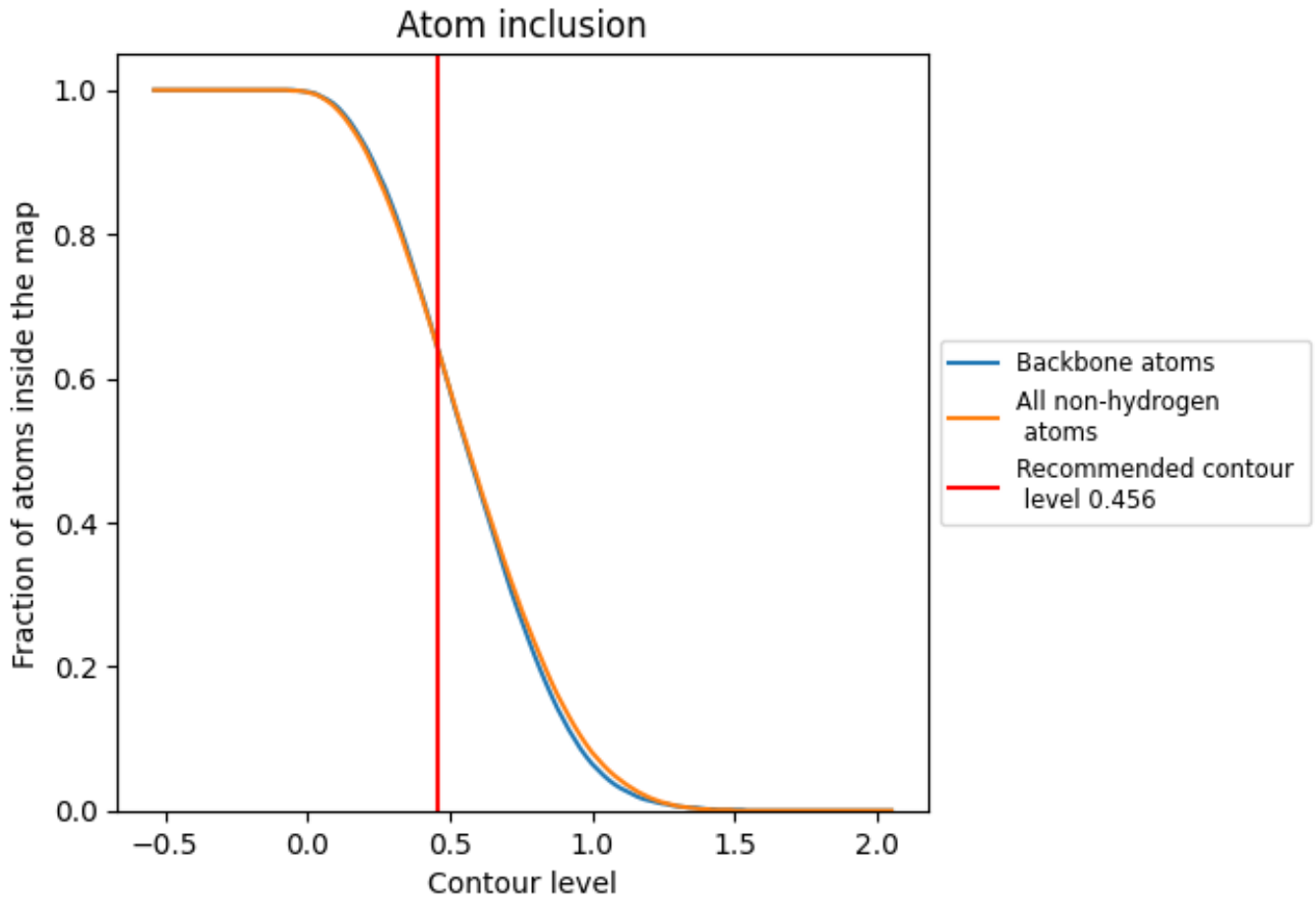
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.456).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.456) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6430	0.4620
1	0.8080	0.5000
2	0.6650	0.4590
4	0.7880	0.4770
5	0.5690	0.4450
6	0.0090	0.1280
7	0.6110	0.5150
A	0.1290	0.2710
B	0.7040	0.5240
C	0.7190	0.5240
D	0.5430	0.4760
E	0.3950	0.4040
F	0.2630	0.3890
G	0.0210	0.2140
H	0.0000	0.0060
I	0.0000	0.0390
J	0.7260	0.5160
K	0.6530	0.5250
L	0.6630	0.5120
M	0.6770	0.5130
N	0.7540	0.5430
O	0.5620	0.4560
P	0.6340	0.5150
Q	0.7650	0.5350
R	0.6260	0.4970
S	0.6790	0.5270
T	0.5780	0.4530
U	0.4810	0.4410
V	0.5530	0.4580
W	0.7090	0.5270
X	0.6640	0.4970
Y	0.5190	0.4010
Z	0.6610	0.5040
a	0.1500	0.3340
b	0.6950	0.5290

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Chain	Atom inclusion	Q-score
c	0.5550	0.4710
d	0.7550	0.5340
e	0.7540	0.5600
f	0.6430	0.4920
g	0.0580	0.3330
h	0.3410	0.4390
i	0.3630	0.4250
j	0.5070	0.4710
k	0.3020	0.4070
l	0.2090	0.3670
m	0.4850	0.4530
n	0.2710	0.3790
o	0.1920	0.3570
p	0.4140	0.4390
q	0.4640	0.4720
r	0.3270	0.4180
s	0.3860	0.4230
t	0.4880	0.4280
u	0.4390	0.4460
v	0.4050	0.3980
w	0.3940	0.3960
x	0.2940	0.3890
y	0.4390	0.4120
z	0.0570	0.3520