Full wwPDB EM Validation Report

Oct 13, 2024 – 01:32 PM EDT

PDB ID	:	7SS9
EMDB ID	:	EMD-25405
Title	:	Late translocation intermediate with EF-G partially dissociated (Structure V)
Authors	:	Carbone, C.E.; Loveland, A.B.; Gamper, H.B.; Hou, Y.; Korostelev, A.A.
Deposited on	:	2021-11-10
Resolution	:	3.90 Å(reported)
Based on initial models	:	?, 5U9F

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

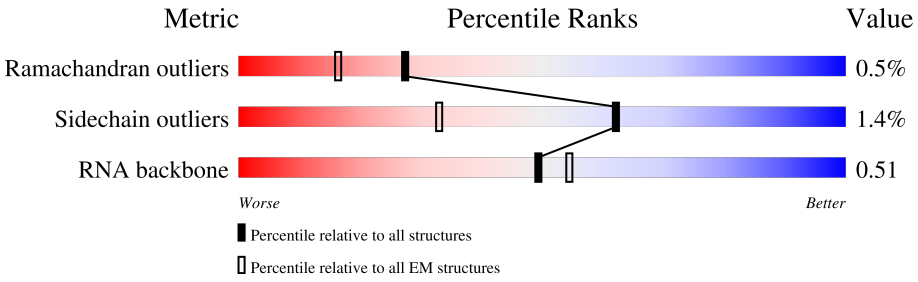
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 3.90 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.



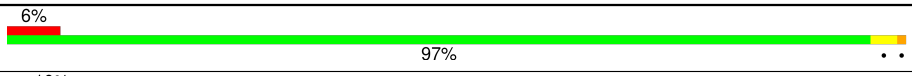
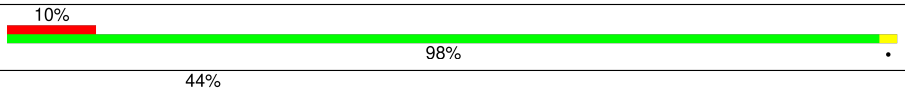
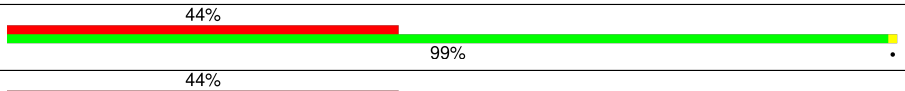
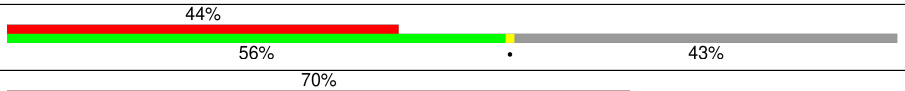
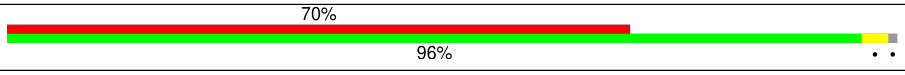
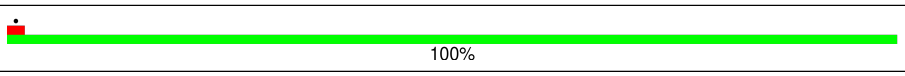
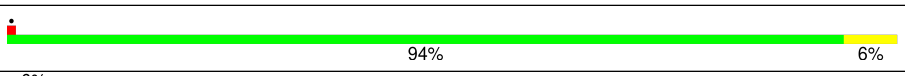
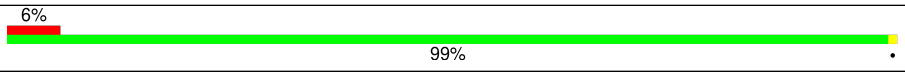
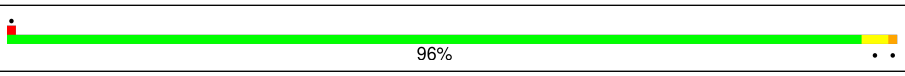
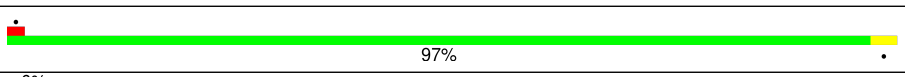
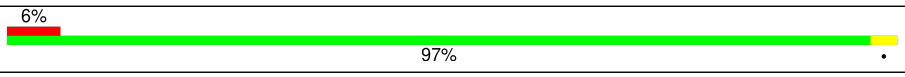
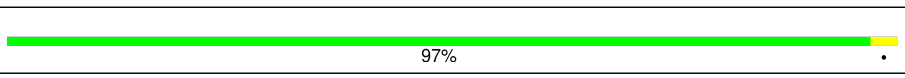
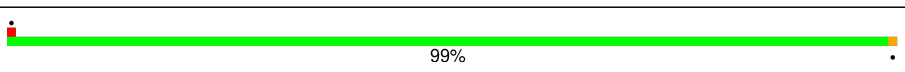
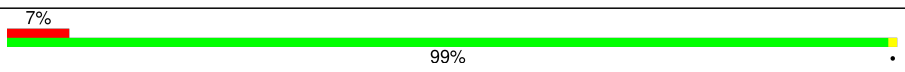
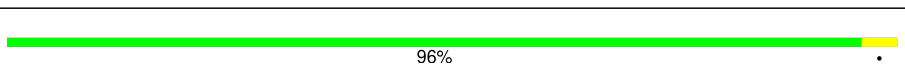
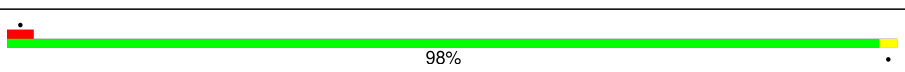
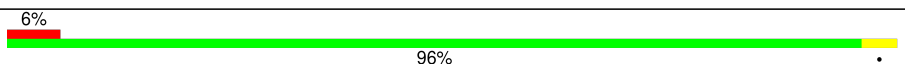
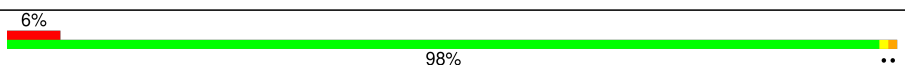
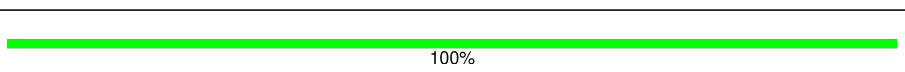
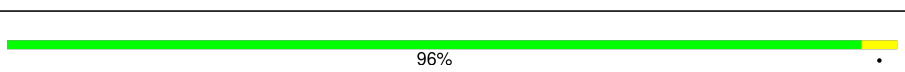
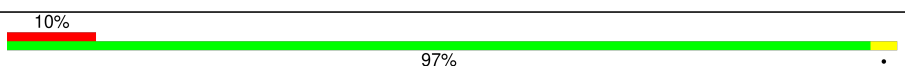
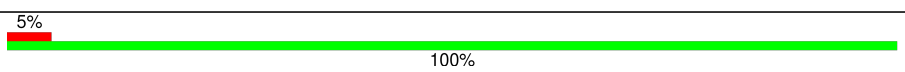
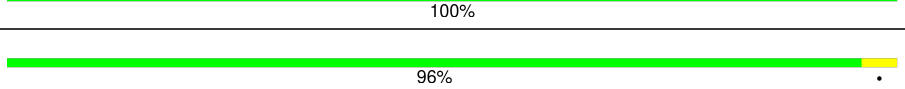
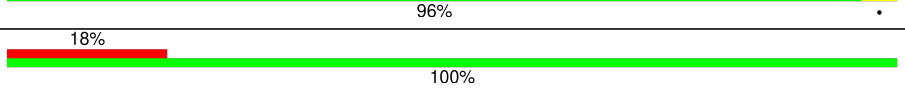
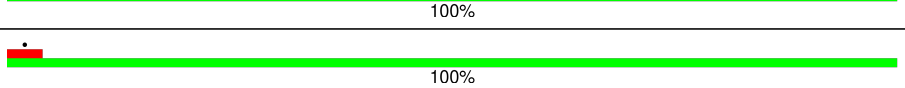
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	3	1539	9% 80% 19%
2	1	2903	80% 20%
3	2	120	86% 14%
4	8	697	19% 40% 59%
5	6	77	43% 77% 22%
6	b	271	97%
7	c	209	99%
8	d	201	6% 99%

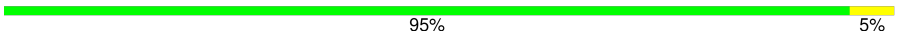
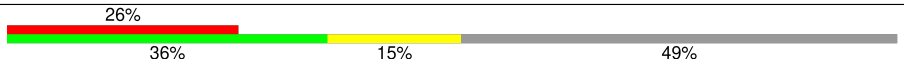
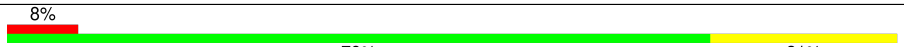
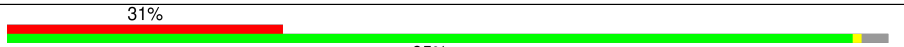
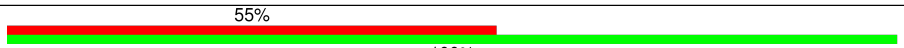
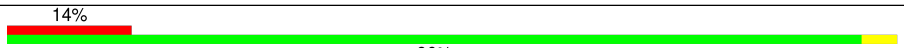
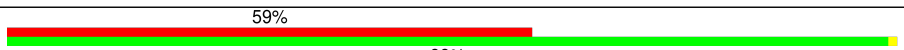
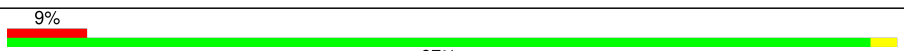
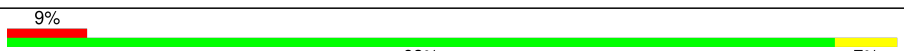
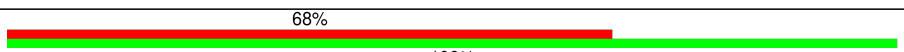
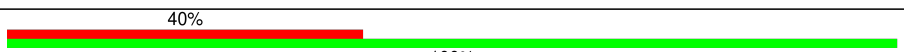
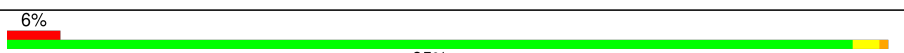
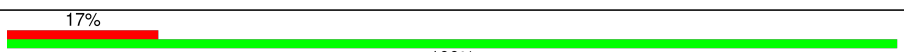
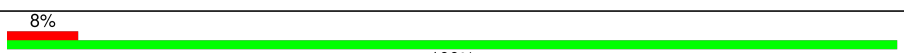
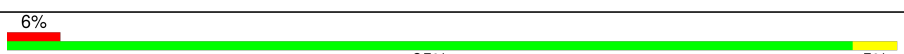
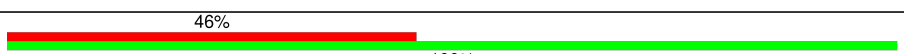
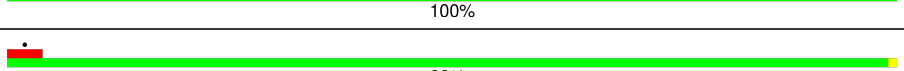
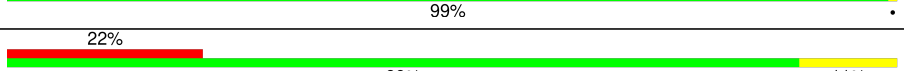
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	e	177	
10	f	176	
11	g	149	
12	a	234	
13	i	142	
14	j	142	
15	k	122	
16	l	143	
17	m	136	
18	n	120	
19	o	116	
20	p	114	
21	q	117	
22	r	103	
23	s	110	
24	t	93	
25	u	102	
26	v	94	
27	w	75	
28	x	77	
29	y	63	
30	z	58	
31	B	56	
32	C	50	
33	D	46	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	E	64	
35	F	38	
36	4	39	
37	5	77	
38	G	225	
39	H	206	
40	I	205	
41	J	157	
42	K	100	
43	L	151	
44	M	129	
45	N	127	
46	O	98	
47	P	116	
48	Q	123	
49	R	114	
50	S	100	
51	T	88	
52	U	82	
53	V	80	
54	W	65	
55	X	79	
56	Y	85	
57	Z	65	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 149808 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	3	1539	33012	14725	6052	10697	1538	0	0

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1	2903	62317	27801	11468	20146	2902	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	120	2568	1145	471	833	119	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	8	286	2213	1401	379	424	9	0	0

- Molecule 5 is a RNA chain called tRNA fMet.

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

- Molecule 6 is a protein called 50S ribosomal protein L2.

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

- Molecule 7 is a protein called 50S ribosomal protein L3.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

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

- Molecule 10 is a protein called 50S ribosomal protein L6.

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

- Molecule 11 is a protein called 50S ribosomal protein L9.

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

- Molecule 12 is a protein called 50S ribosomal protein L1.

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

- Molecule 13 is a protein called 50S ribosomal protein L11.

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

- Molecule 14 is a protein called 50S ribosomal protein L13.

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

- Molecule 15 is a protein called 50S ribosomal protein L14.

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

- Molecule 16 is a protein called 50S ribosomal protein L15.

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

- Molecule 17 is a protein called 50S ribosomal protein L16.

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

- Molecule 18 is a protein called 50S ribosomal protein L17.

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

- Molecule 19 is a protein called 50S ribosomal protein L18.

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

- Molecule 20 is a protein called 50S ribosomal protein L19.

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

- Molecule 21 is a protein called 50S ribosomal protein L20.

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

- Molecule 22 is a protein called 50S ribosomal protein L21.

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

- Molecule 23 is a protein called 50S ribosomal protein L22.

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

- Molecule 24 is a protein called 50S ribosomal protein L23.

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

- Molecule 25 is a protein called 50S ribosomal protein L24.

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

- Molecule 26 is a protein called 50S ribosomal protein L25.

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

- Molecule 27 is a protein called 50S ribosomal protein L27.

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

- Molecule 28 is a protein called 50S ribosomal protein L28.

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

- Molecule 29 is a protein called 50S ribosomal protein L29.

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L33.

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

- Molecule 33 is a protein called 50S ribosomal protein L34.

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

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L36.

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

- Molecule 36 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	4	20	Total	C	N	O	P	0	0
			436	195	87	134	20		

- Molecule 37 is a RNA chain called tRNA Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	5	77	Total	C	N	O	P	0	0
			1647	733	295	542	77		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	G	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	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 30S ribosomal protein S5.

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

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

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

- 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
			1182	735	227	216	4		

- Molecule 44 is a protein called 30S ribosomal protein S8.

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 30S ribosomal protein S9.

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 30S ribosomal protein S10.

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

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

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

- Molecule 48 is a protein called 30S ribosomal protein S12.

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

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

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

- Molecule 50 is a protein called 30S ribosomal protein S14.

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 30S ribosomal protein S15.

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 30S ribosomal protein S17.

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

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

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

- Molecule 55 is a protein called 30S ribosomal protein S19.

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

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

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

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

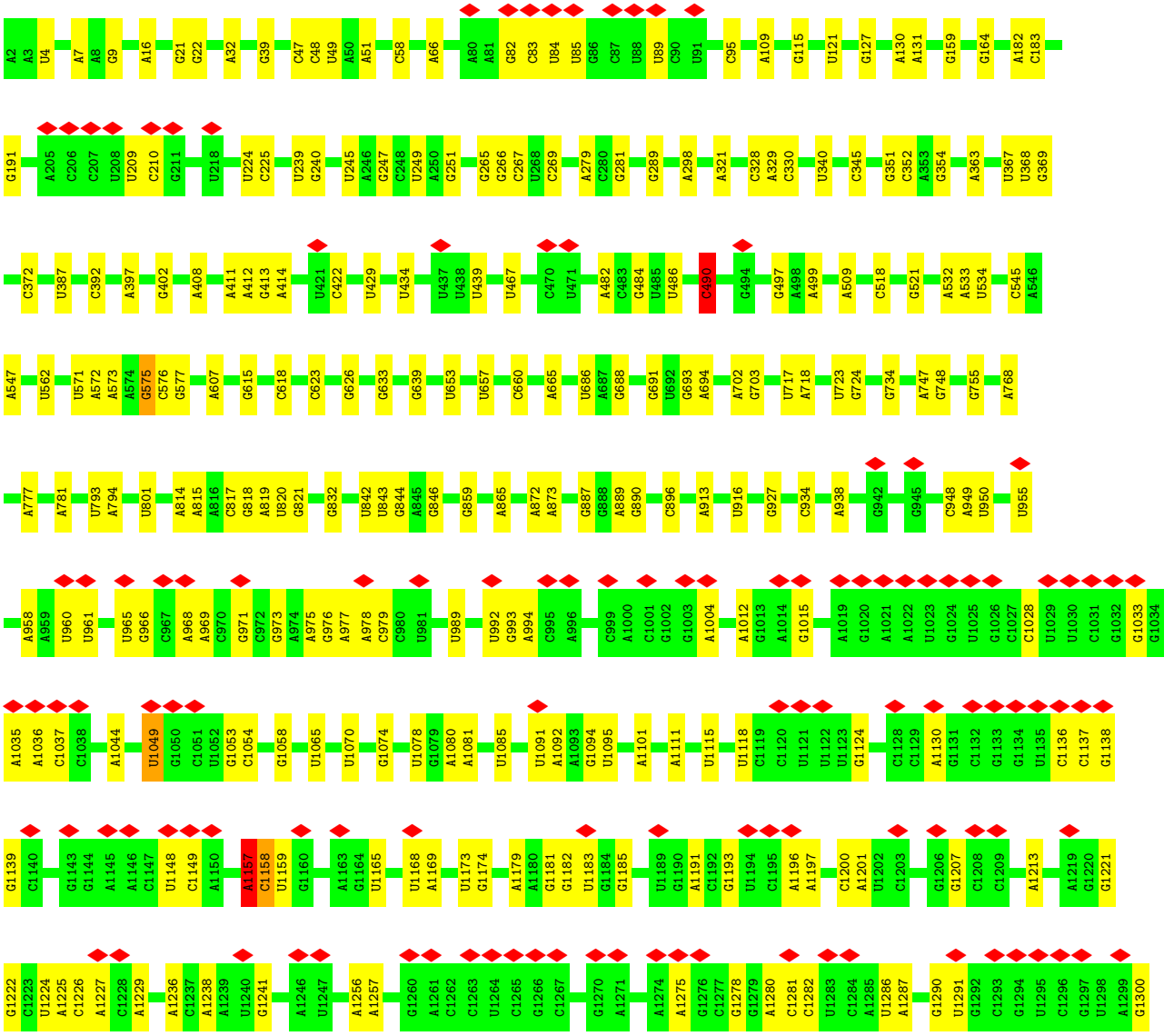
Mol	Chain	Residues	Atoms					AltConf	Trace
57	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

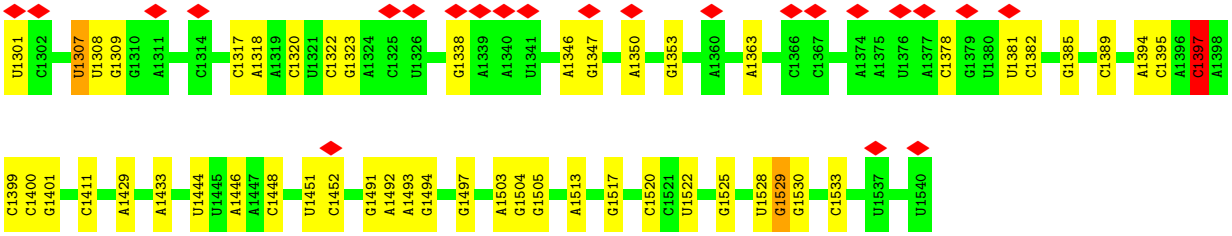
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

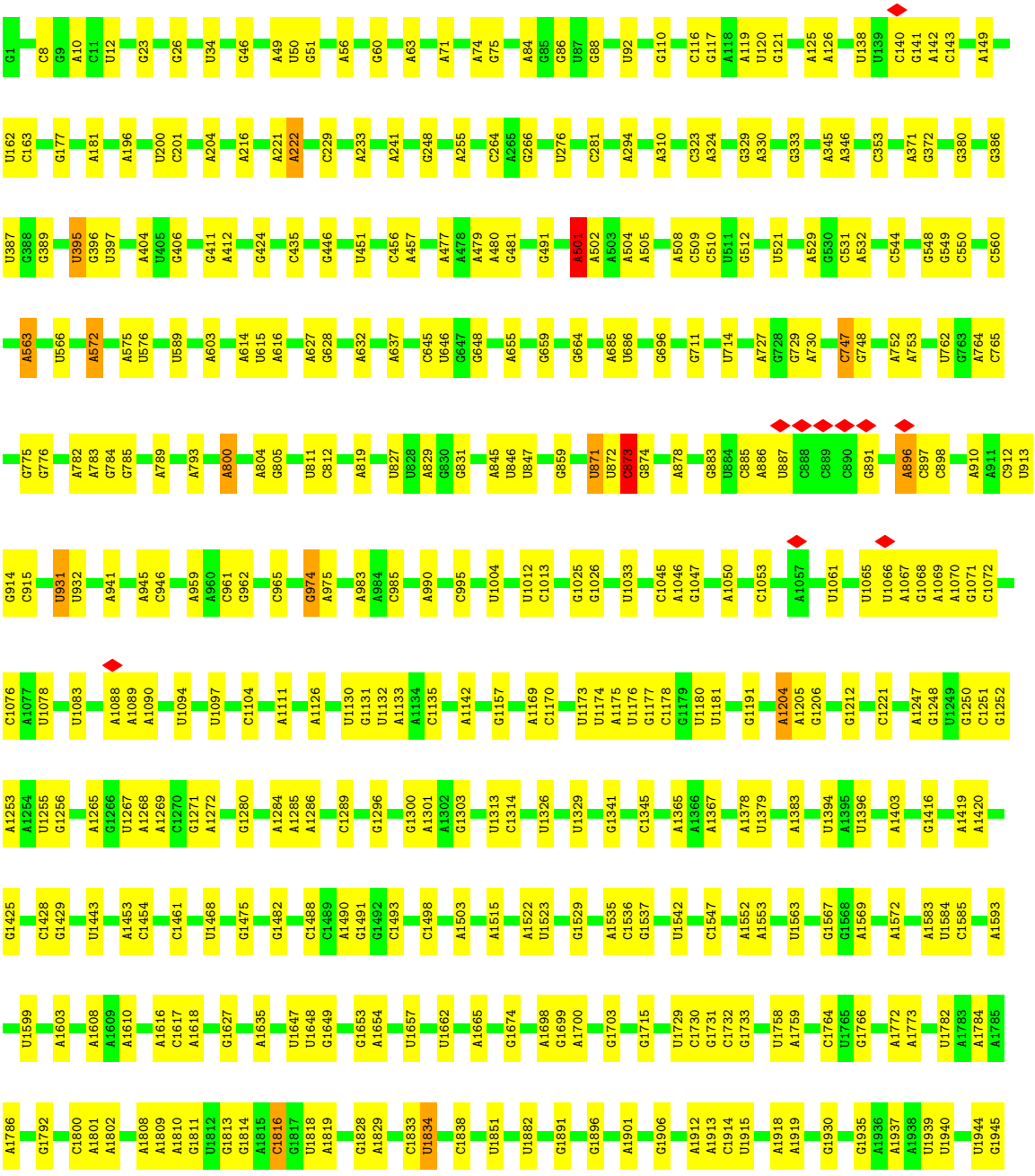
Chain 3:

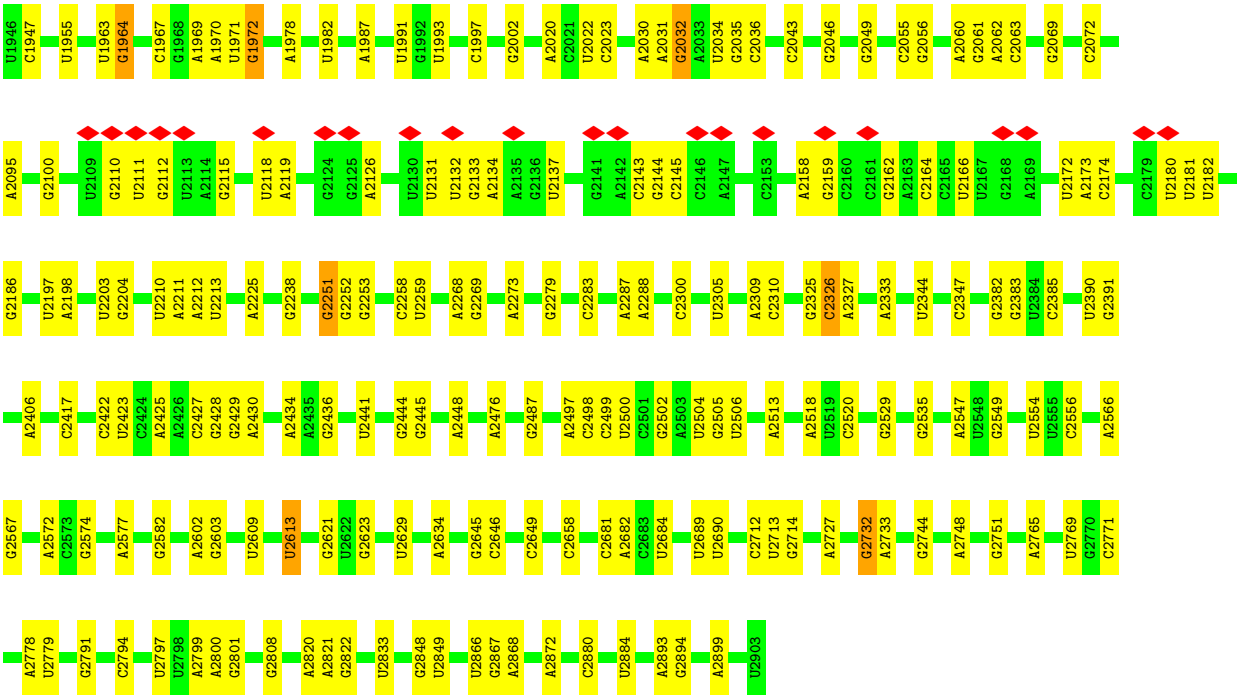




• Molecule 2: 23S rRNA

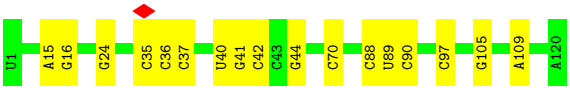
Chain 1:





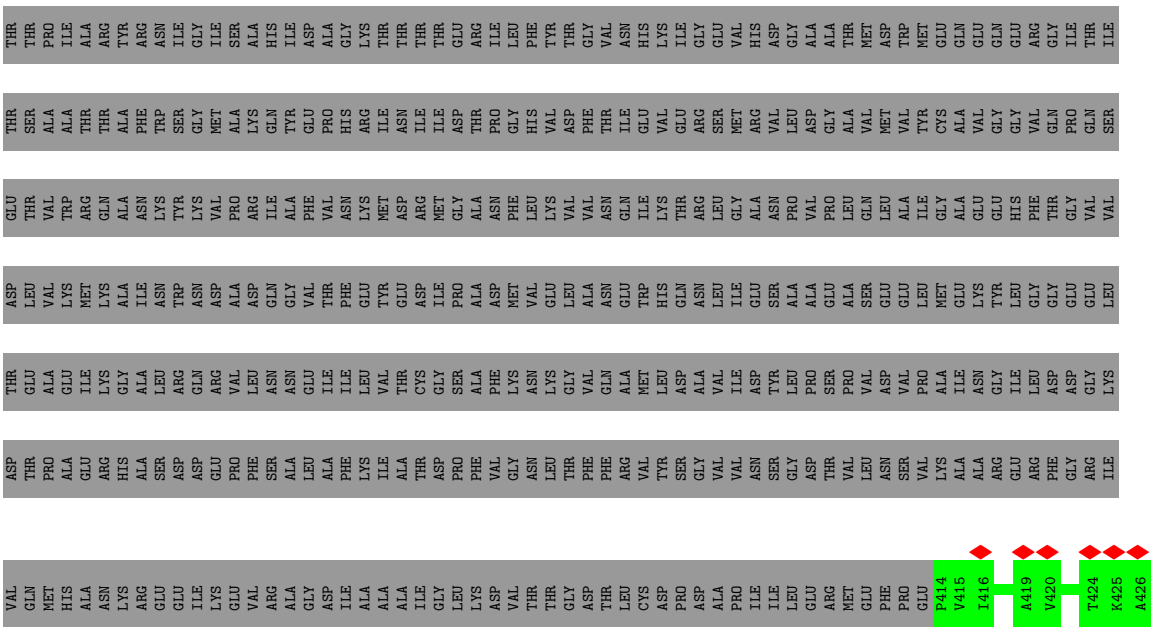
• Molecule 3: 5S rRNA

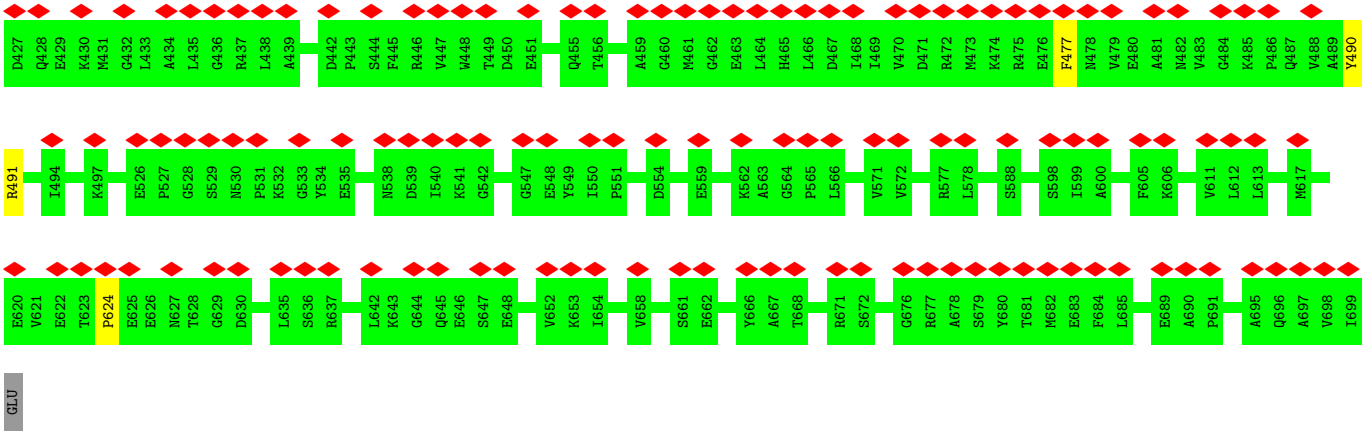
Chain 2:



• Molecule 4: Elongation factor G

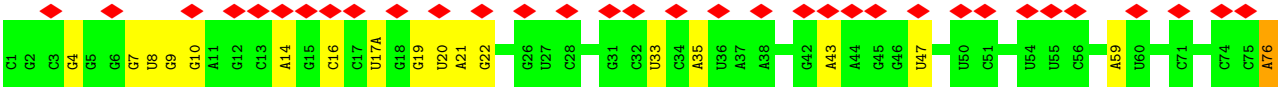
Chain 8:





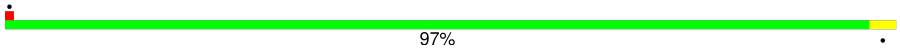
• Molecule 5: tRNA fMet

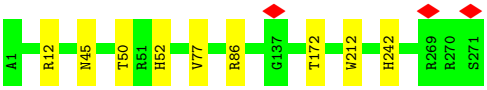
Chain 6:



• Molecule 6: 50S ribosomal protein L2

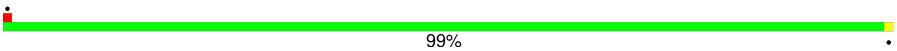
Chain b:





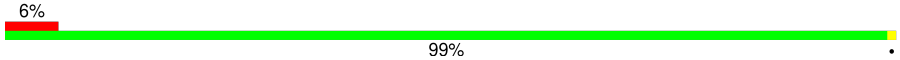
• Molecule 7: 50S ribosomal protein L3

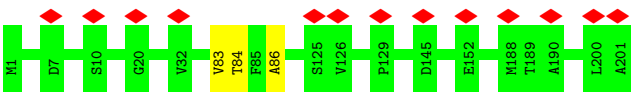
Chain c:



• Molecule 8: 50S ribosomal protein L4

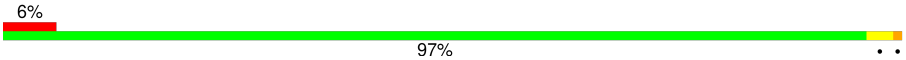
Chain d:

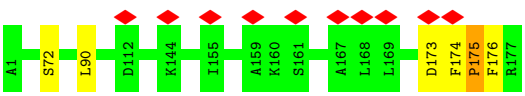




• Molecule 9: 50S ribosomal protein L5

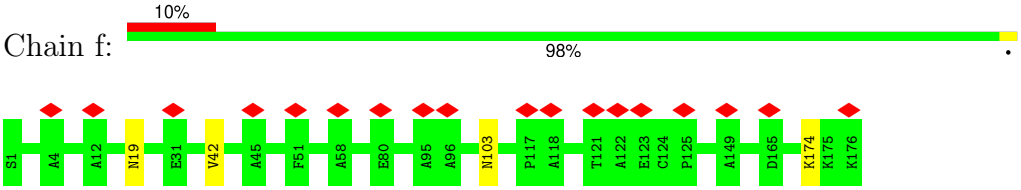
Chain e:





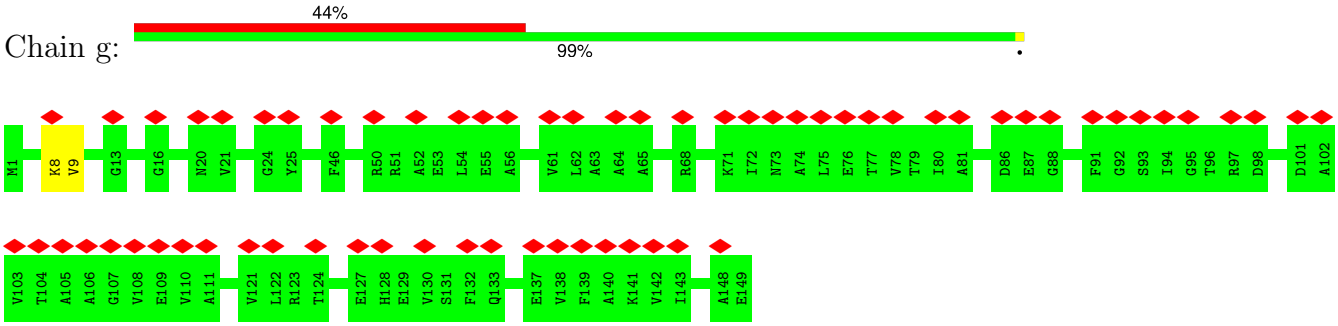
• Molecule 10: 50S ribosomal protein L6

Chain f:



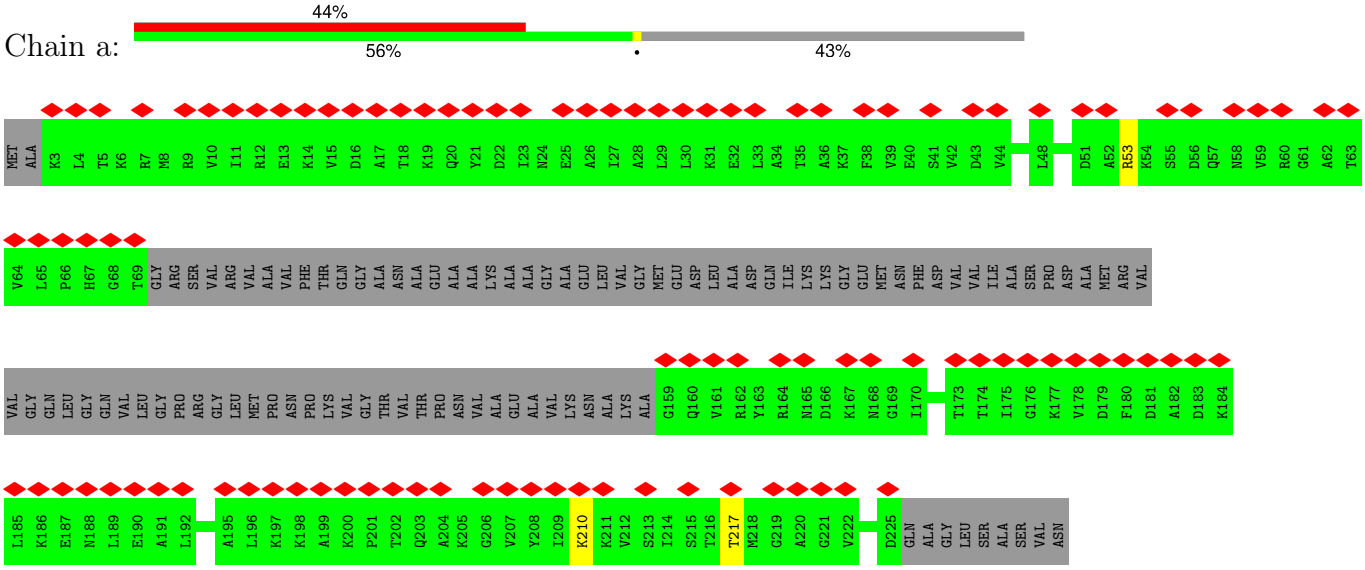
• Molecule 11: 50S ribosomal protein L9

Chain g:



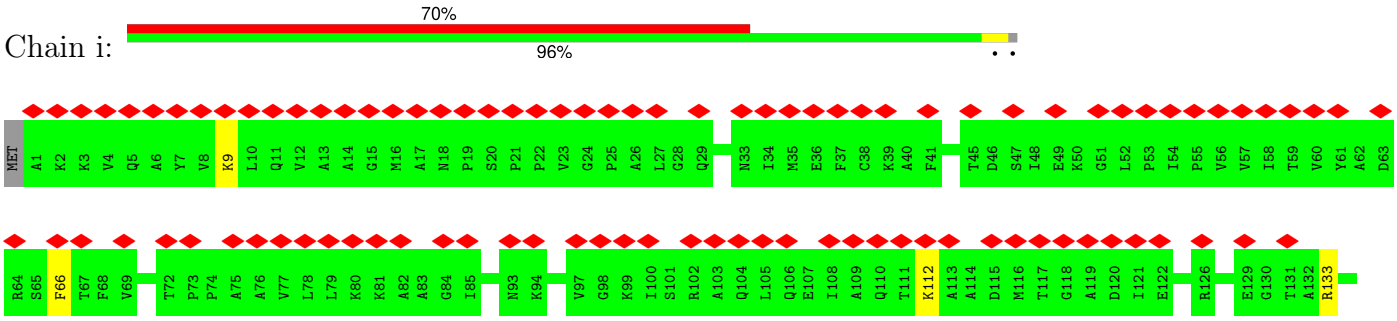
• Molecule 12: 50S ribosomal protein L1

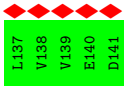
Chain a:



• Molecule 13: 50S ribosomal protein L11

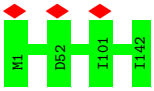
Chain i:





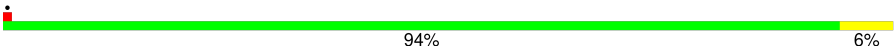
• Molecule 14: 50S ribosomal protein L13

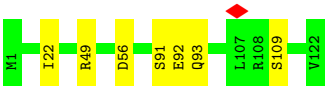
Chain j:



• Molecule 15: 50S ribosomal protein L14

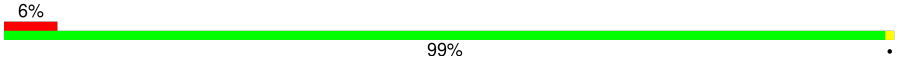
Chain k:

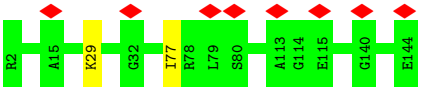




• Molecule 16: 50S ribosomal protein L15

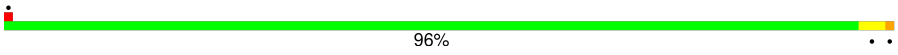
Chain l:

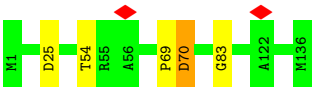




• Molecule 17: 50S ribosomal protein L16

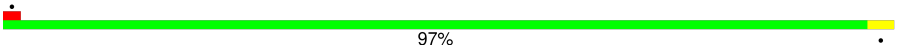
Chain m:

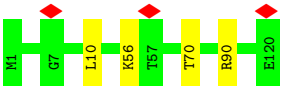




• Molecule 18: 50S ribosomal protein L17

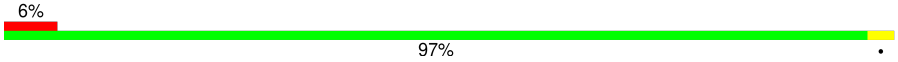
Chain n:

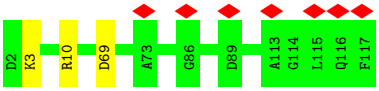




• Molecule 19: 50S ribosomal protein L18

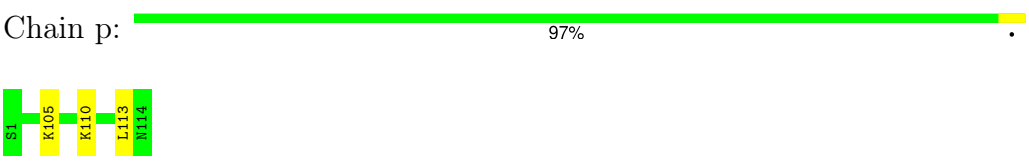
Chain o:





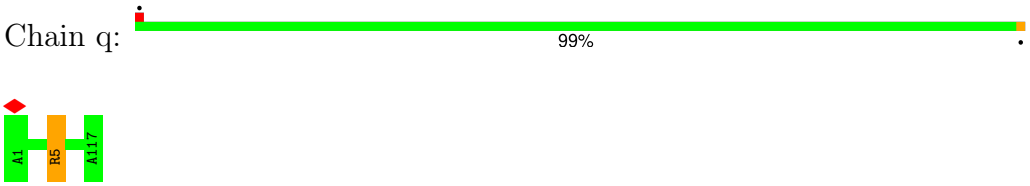
• Molecule 20: 50S ribosomal protein L19

Chain p:



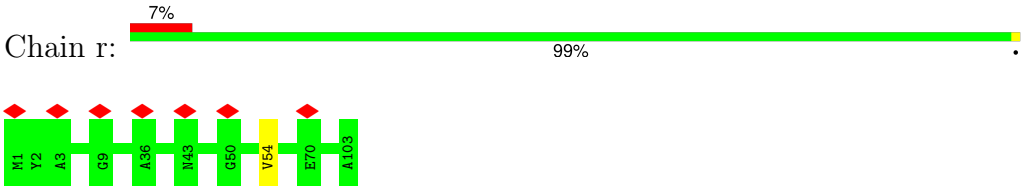
• Molecule 21: 50S ribosomal protein L20

Chain q:



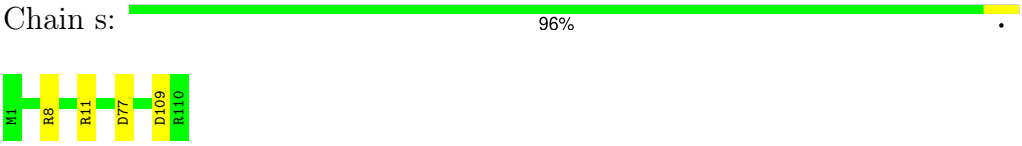
• Molecule 22: 50S ribosomal protein L21

Chain r:



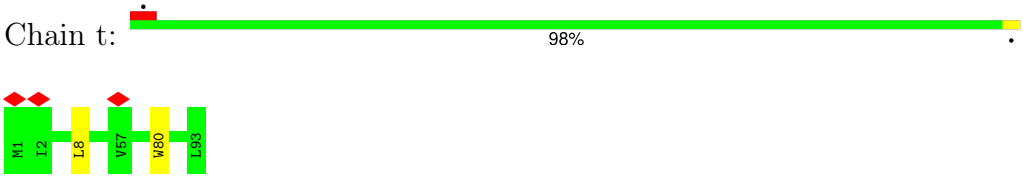
• Molecule 23: 50S ribosomal protein L22

Chain s:



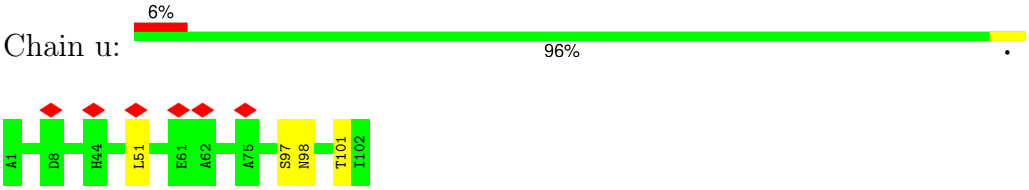
• Molecule 24: 50S ribosomal protein L23

Chain t:



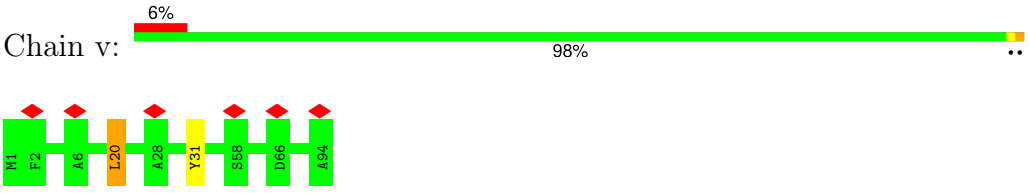
• Molecule 25: 50S ribosomal protein L24

Chain u:



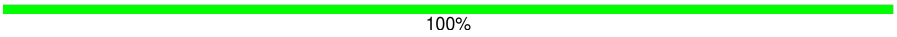
• Molecule 26: 50S ribosomal protein L25

Chain v:



• Molecule 27: 50S ribosomal protein L27

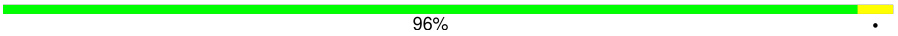
Chain w:

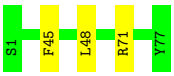


There are no outlier residues recorded for this chain.

• Molecule 28: 50S ribosomal protein L28

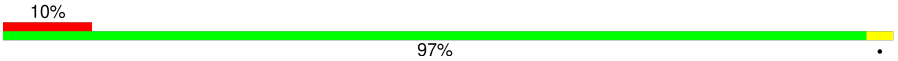
Chain x:

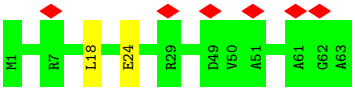




• Molecule 29: 50S ribosomal protein L29

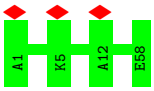
Chain y:





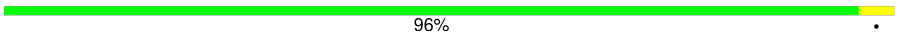
• Molecule 30: 50S ribosomal protein L30

Chain z:



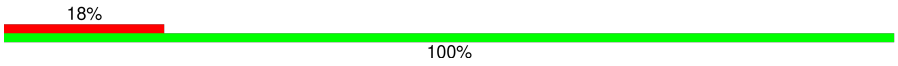
• Molecule 31: 50S ribosomal protein L32

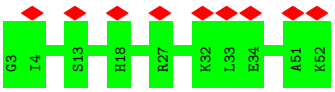
Chain B:



• Molecule 32: 50S ribosomal protein L33

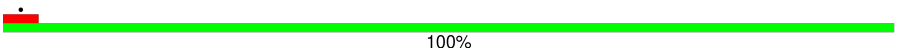
Chain C:

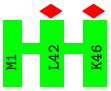




• Molecule 33: 50S ribosomal protein L34

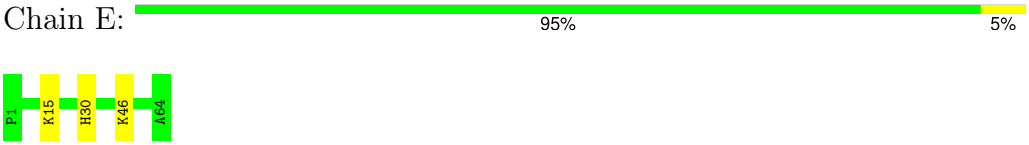
Chain D:





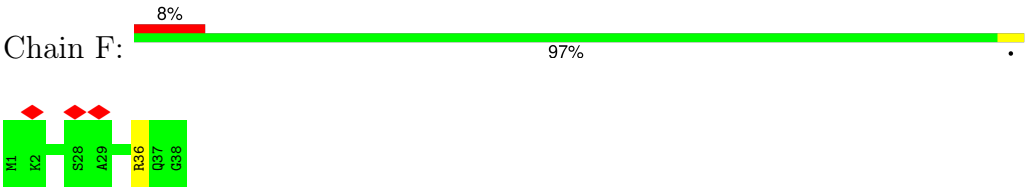
• Molecule 34: 50S ribosomal protein L35

Chain E:



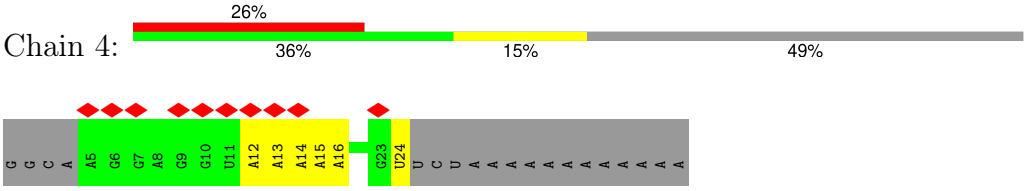
• Molecule 35: 50S ribosomal protein L36

Chain F:



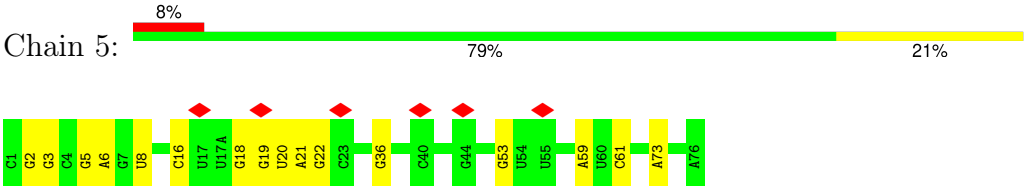
• Molecule 36: mRNA

Chain 4:



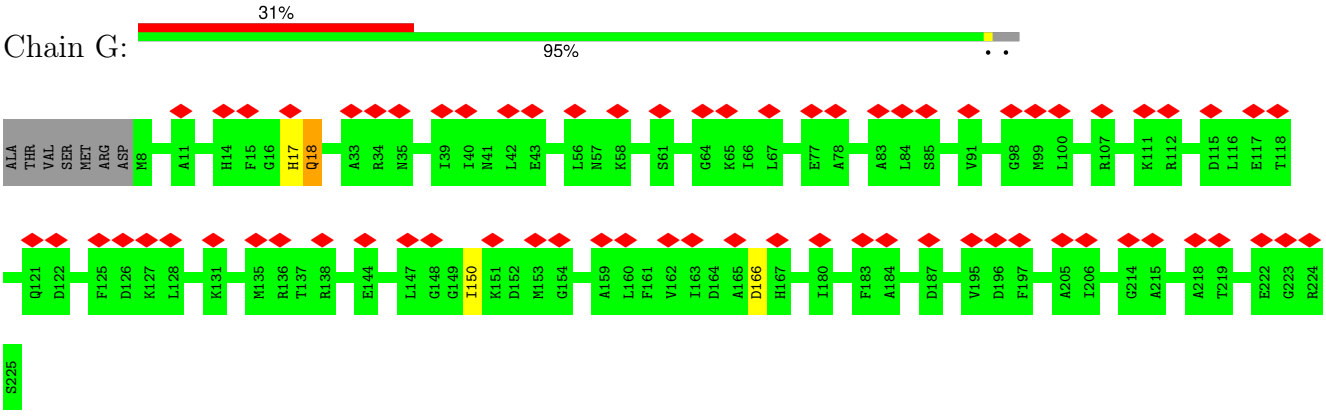
• Molecule 37: tRNA Pro

Chain 5:



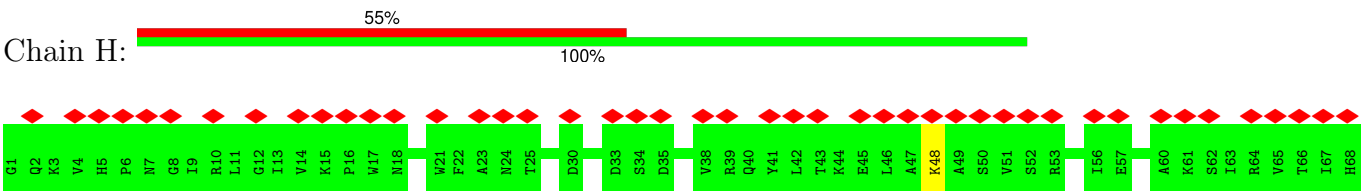
• Molecule 38: 30S ribosomal protein S2

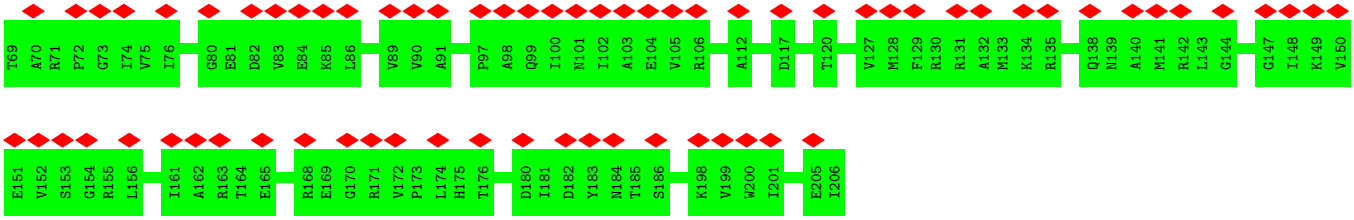
Chain G:



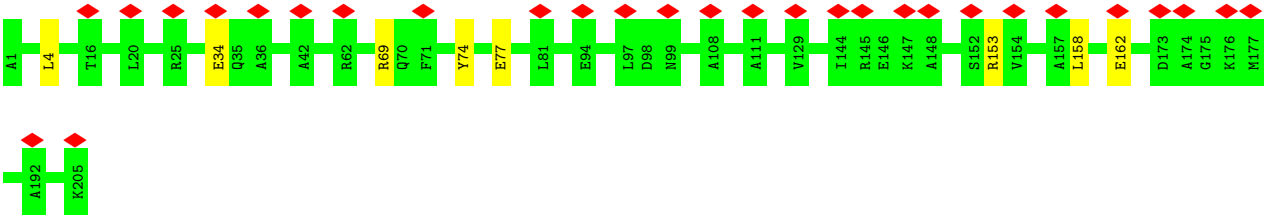
• Molecule 39: 30S ribosomal protein S3

Chain H:

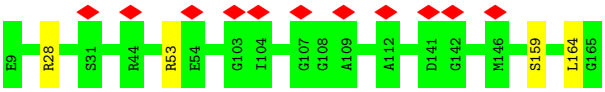




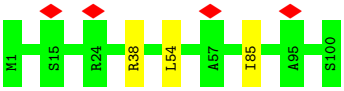
• Molecule 40: 30S ribosomal protein S4



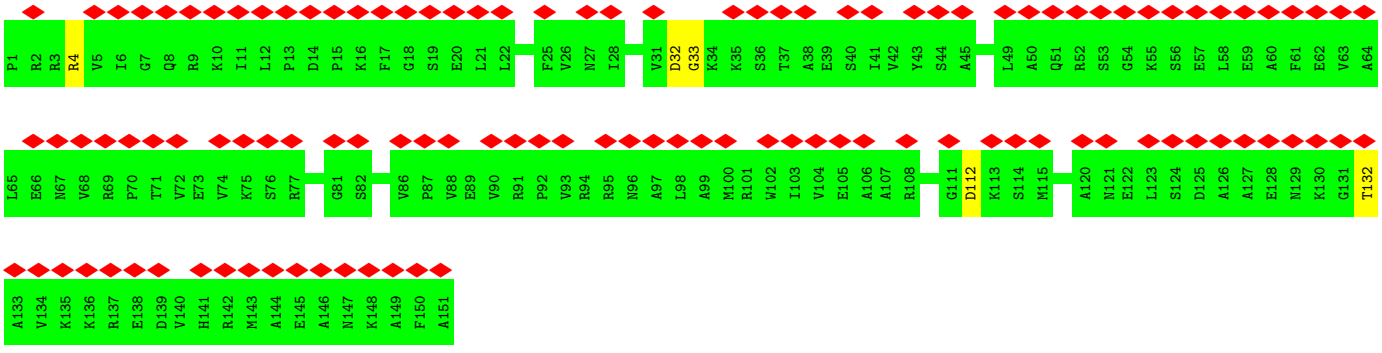
• Molecule 41: 30S ribosomal protein S5



• Molecule 42: 30S ribosomal protein S6

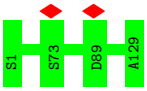


• Molecule 43: 30S ribosomal protein S7



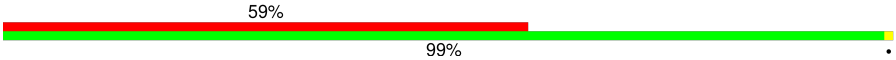
• Molecule 44: 30S ribosomal protein S8

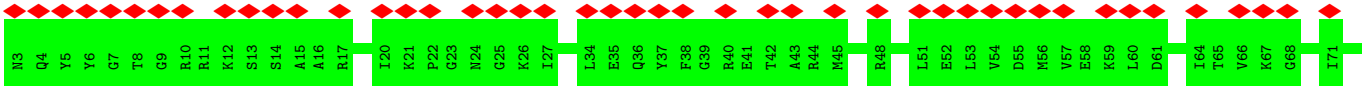
Chain M:

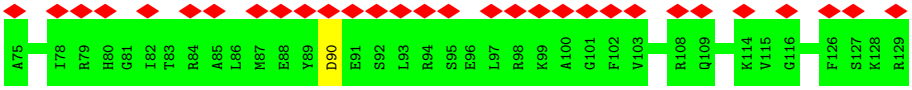


• Molecule 45: 30S ribosomal protein S9

Chain N:

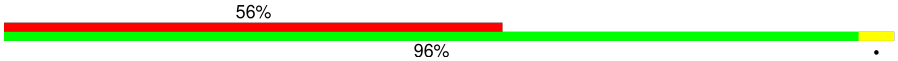


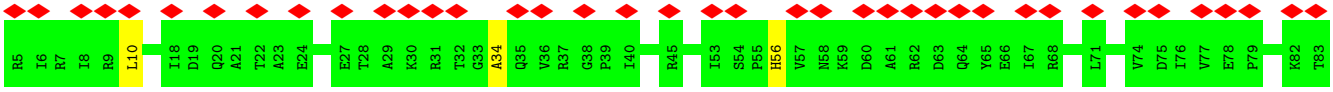


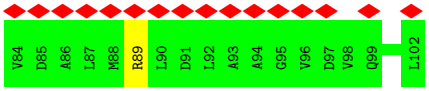


• Molecule 46: 30S ribosomal protein S10

Chain O:

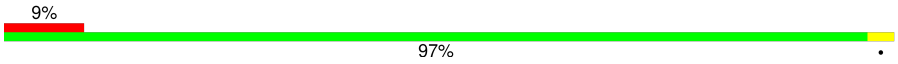


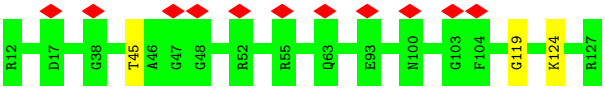




• Molecule 47: 30S ribosomal protein S11

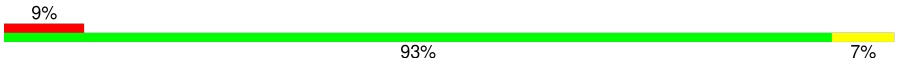
Chain P:

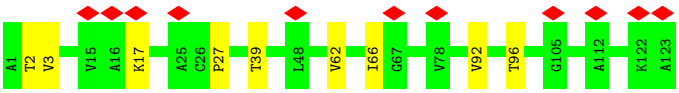




• Molecule 48: 30S ribosomal protein S12

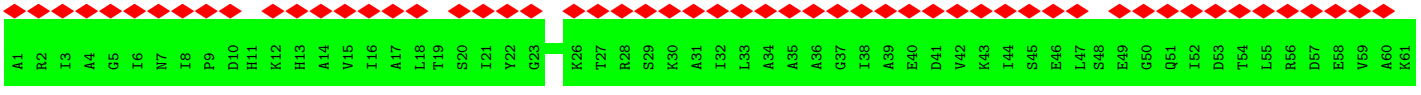
Chain Q:

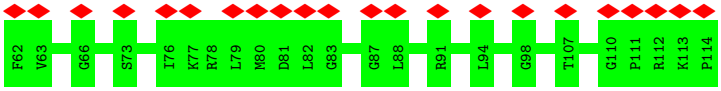




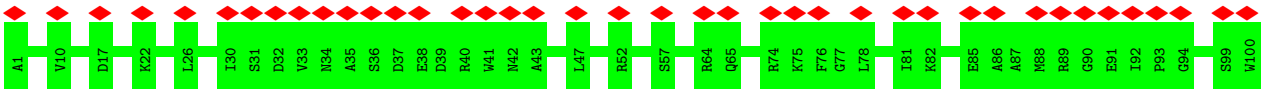
• Molecule 49: 30S ribosomal protein S13

Chain R:

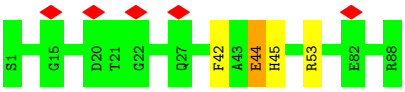




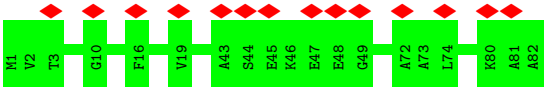
• Molecule 50: 30S ribosomal protein S14



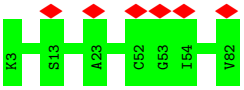
• Molecule 51: 30S ribosomal protein S15



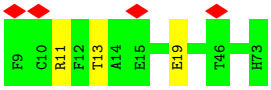
• Molecule 52: 30S ribosomal protein S16



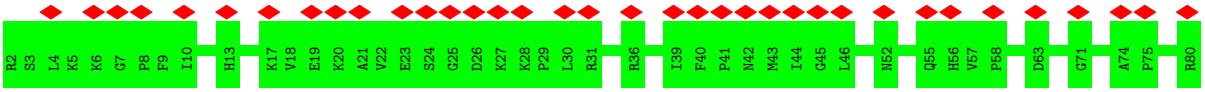
• Molecule 53: 30S ribosomal protein S17



• Molecule 54: 30S ribosomal protein S18

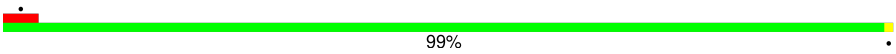


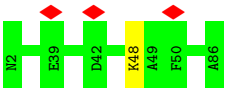
• Molecule 55: 30S ribosomal protein S19



• Molecule 56: 30S ribosomal protein S20

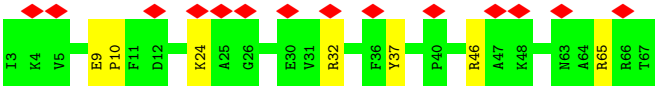
Chain Y:





• 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	1105	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 ($e^-/Å^2$)	47.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	18.334	Depositor
Minimum map value	-12.168	Depositor
Average map value	0.114	Depositor
Map value standard deviation	0.809	Depositor
Recommended contour level	1.75	Depositor
Map size (Å)	370.5408, 370.5408, 370.5408	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8271, 0.8271, 0.8271	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	3	0.72	2/36963 (0.0%)	0.72	11/57662 (0.0%)
2	1	0.71	1/69796 (0.0%)	0.72	18/108888 (0.0%)
3	2	0.66	0/2872	0.71	0/4479
4	8	0.34	0/2255	0.64	0/3040
5	6	0.82	0/1832	0.73	1/2855 (0.0%)
6	b	0.54	0/2122	0.74	1/2852 (0.0%)
7	c	0.52	0/1586	0.69	0/2134
8	d	0.46	0/1571	0.66	0/2113
9	e	0.39	0/1435	0.69	1/1926 (0.1%)
10	f	0.38	0/1343	0.63	0/1816
11	g	0.37	0/1122	0.66	0/1515
12	a	0.30	0/1033	0.64	0/1387
13	i	0.34	0/1046	0.64	0/1410
14	j	0.50	0/1152	0.62	0/1551
15	k	0.54	0/948	0.75	0/1268
16	l	0.49	0/1054	0.71	0/1403
17	m	0.51	0/1093	0.66	0/1460
18	n	0.54	0/974	0.71	0/1301
19	o	0.41	0/902	0.62	0/1209
20	p	0.47	0/929	0.66	1/1242 (0.1%)
21	q	0.55	0/960	0.62	1/1278 (0.1%)
22	r	0.45	0/829	0.63	0/1107
23	s	0.46	0/864	0.67	0/1156
24	t	0.44	0/745	0.64	1/994 (0.1%)
25	u	0.44	0/788	0.68	1/1051 (0.1%)
26	v	0.40	0/766	0.62	1/1025 (0.1%)
27	w	0.49	0/582	0.68	0/769
28	x	0.50	0/635	0.71	1/848 (0.1%)
29	y	0.38	0/510	0.70	1/677 (0.1%)
30	z	0.42	0/453	0.66	0/605
31	B	0.46	0/450	0.68	0/599
32	C	0.40	0/417	0.65	0/554
33	D	0.50	0/380	0.67	0/498
34	E	0.51	0/513	0.70	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	F	0.47	0/303	0.68	0/397
36	4	0.79	0/490	0.76	0/763
37	5	0.79	0/1840	0.71	0/2868
38	G	0.38	0/1736	0.66	0/2338
39	H	0.32	0/1652	0.59	0/2225
40	I	0.39	0/1665	0.68	0/2227
41	J	0.44	0/1170	0.77	1/1573 (0.1%)
42	K	0.45	0/836	0.71	1/1128 (0.1%)
43	L	0.32	0/1196	0.61	0/1602
44	M	0.42	0/989	0.68	0/1326
45	N	0.34	0/1034	0.69	0/1375
46	O	0.36	0/797	0.73	1/1077 (0.1%)
47	P	0.37	0/886	0.67	0/1195
48	Q	0.47	0/969	0.76	0/1300
49	R	0.32	0/893	0.64	0/1193
50	S	0.36	0/817	0.67	0/1088
51	T	0.38	0/722	0.65	0/964
52	U	0.43	0/659	0.67	0/884
53	V	0.43	0/658	0.65	0/881
54	W	0.38	0/545	0.68	0/731
55	X	0.36	0/653	0.66	0/877
56	Y	0.33	0/671	0.58	0/888
57	Z	0.45	0/551	0.91	0/728
All	All	0.64	3/162652 (0.0%)	0.71	42/242976 (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	3	0	11
2	1	1	26
4	8	0	1
5	6	0	1
6	b	0	3
7	c	0	1
8	d	0	1
9	e	0	2
10	f	0	1
11	g	0	1
13	i	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
15	k	0	4
16	l	0	1
17	m	0	3
18	n	0	1
23	s	0	1
25	u	0	1
34	E	0	1
35	F	0	1
36	4	1	0
38	G	0	2
40	I	0	1
41	J	0	1
43	L	0	1
46	O	0	1
47	P	0	1
48	Q	0	2
51	T	0	1
54	W	0	1
All	All	2	73

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	1816	C	N1-C2	5.29	1.45	1.40
1	3	1158	C	N1-C2	5.23	1.45	1.40
1	3	1049	U	C4-C5	5.04	1.48	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3	1307	U	O4'-C1'-N1	9.05	115.44	108.20
2	1	873	C	O4'-C1'-N1	8.81	115.25	108.20
2	1	873	C	N1-C1'-C2'	8.29	124.78	114.00
1	3	1397	C	N1-C1'-C2'	-8.07	103.12	112.00
2	1	1944	U	N1-C1'-C2'	8.03	124.44	114.00
20	p	113	LEU	CA-CB-CG	7.50	132.55	115.30
2	1	2430	A	N9-C1'-C2'	7.24	123.41	114.00
1	3	950	U	O4'-C1'-N1	7.00	113.80	108.20
25	u	51	LEU	CA-CB-CG	6.73	130.77	115.30
29	y	18	LEU	CA-CB-CG	6.40	130.02	115.30
1	3	1307	U	C5'-C4'-C3'	6.24	125.99	116.00
26	v	20	LEU	CA-CB-CG	6.06	129.24	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	J	164	LEU	CA-CB-CG	6.03	129.17	115.30
46	O	10	LEU	CA-CB-CG	6.02	129.15	115.30
1	3	1307	U	C1'-O4'-C4'	-5.90	105.18	109.90
2	1	2251	G	N9-C1'-C2'	5.82	121.57	114.00
2	1	1818	U	N1-C1'-C2'	5.76	121.48	114.00
2	1	2506	U	N1-C1'-C2'	5.69	121.40	114.00
2	1	395	U	N1-C1'-C2'	5.61	121.30	114.00
6	b	12	ARG	CA-CB-CG	5.42	125.33	113.40
2	1	501	A	N9-C1'-C2'	5.38	120.99	114.00
2	1	871	U	N1-C1'-C2'	5.37	120.97	114.00
42	K	54	LEU	CA-CB-CG	5.36	127.62	115.30
2	1	563	A	N9-C1'-C2'	5.34	120.94	114.00
1	3	950	U	O4'-C4'-C3'	-5.34	98.66	104.00
9	e	90	LEU	CB-CG-CD2	-5.30	102.00	111.00
2	1	2326	C	C2'-C3'-O3'	5.28	122.15	113.70
24	t	8	LEU	CA-CB-CG	-5.28	103.16	115.30
2	1	2032	G	N9-C1'-C2'	5.25	120.82	114.00
2	1	896	A	C2'-C3'-O3'	5.22	122.06	113.70
1	3	1529	G	OP1-P-O3'	5.18	116.60	105.20
2	1	572	A	N9-C1'-C2'	5.14	120.68	114.00
1	3	575	G	N9-C1'-C2'	5.11	120.65	114.00
2	1	931	U	N1-C1'-C2'	5.11	120.64	114.00
5	6	33	U	O4'-C1'-N1	5.10	112.28	108.20
1	3	490	C	N1-C1'-C2'	5.09	120.62	114.00
2	1	974	G	N9-C1'-C2'	5.08	120.60	114.00
28	x	48	LEU	CA-CB-CG	5.07	126.95	115.30
1	3	1157	A	N9-C1'-C2'	5.06	120.58	114.00
2	1	747	C	N1-C1'-C2'	5.04	120.56	114.00
21	q	5	ARG	CA-CB-CG	5.01	124.41	113.40
1	3	686	U	N1-C1'-C2'	5.00	120.50	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	1	873	C	C1'
36	4	13	A	C4'

All (73) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	1025	G	Sidechain
2	1	1191	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	1	1204	A	Sidechain
2	1	1425	G	Sidechain
2	1	1792	G	Sidechain
2	1	1814	G	Sidechain
2	1	1828	G	Sidechain
2	1	1834	U	Sidechain
2	1	1964	G	Sidechain
2	1	1972	G	Sidechain
2	1	2180	U	Sidechain
2	1	222	A	Sidechain
2	1	2273	A	Sidechain
2	1	2344	U	Sidechain
2	1	2582	G	Sidechain
2	1	26	G	Sidechain
2	1	2613	U	Sidechain
2	1	2732	G	Sidechain
2	1	2769	U	Sidechain
2	1	477	A	Sidechain
2	1	501	A	Sidechain
2	1	566	U	Sidechain
2	1	576	U	Sidechain
2	1	727	A	Sidechain
2	1	800	A	Sidechain
2	1	873	C	Sidechain
1	3	1049	U	Sidechain
1	3	1078	U	Sidechain
1	3	1148	U	Sidechain
1	3	1157	A	Sidechain
1	3	1397	C	Sidechain
1	3	1444	U	Sidechain
1	3	159	G	Sidechain
1	3	490	C	Sidechain
1	3	820	U	Sidechain
1	3	896	C	Sidechain
1	3	948	C	Sidechain
5	6	76	A	Sidechain
4	8	490	TYR	Peptide
34	E	30	HIS	Peptide
35	F	36	ARG	Peptide
38	G	17	HIS	Peptide
38	G	18	GLN	Peptide
40	I	77	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
41	J	159	SER	Peptide
43	L	32	ASP	Peptide
46	O	34	ALA	Peptide
47	P	119	GLY	Peptide
48	Q	2	THR	Peptide
48	Q	92	VAL	Peptide
51	T	44	GLU	Peptide
54	W	19	GLU	Peptide
6	b	242	HIS	Peptide
6	b	45	ASN	Peptide
6	b	86	ARG	Peptide
7	c	159	LYS	Peptide
8	d	83	VAL	Peptide
9	e	174	PHE	Peptide
9	e	175	PRO	Peptide
10	f	174	LYS	Peptide
11	g	8	LYS	Peptide
13	i	9	LYS	Peptide
15	k	109	SER	Peptide
15	k	91	SER	Peptide
15	k	92	GLU	Peptide
15	k	93	GLN	Peptide
16	l	29	LYS	Peptide
17	m	25	ASP	Peptide
17	m	70	ASP	Peptide
17	m	83	GLY	Peptide
18	n	10	LEU	Peptide
23	s	8	ARG	Peptide
25	u	97	SER	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
4	8	284/697 (41%)	241 (85%)	41 (14%)	2 (1%)	19 54
6	b	269/271 (99%)	235 (87%)	34 (13%)	0	100 100
7	c	207/209 (99%)	181 (87%)	26 (13%)	0	100 100
8	d	199/201 (99%)	181 (91%)	17 (8%)	1 (0%)	25 60
9	e	175/177 (99%)	159 (91%)	13 (7%)	3 (2%)	7 36
10	f	174/176 (99%)	163 (94%)	11 (6%)	0	100 100
11	g	147/149 (99%)	129 (88%)	17 (12%)	1 (1%)	19 54
12	a	130/234 (56%)	112 (86%)	17 (13%)	1 (1%)	16 51
13	i	139/142 (98%)	125 (90%)	14 (10%)	0	100 100
14	j	140/142 (99%)	128 (91%)	12 (9%)	0	100 100
15	k	120/122 (98%)	96 (80%)	24 (20%)	0	100 100
16	l	141/143 (99%)	121 (86%)	20 (14%)	0	100 100
17	m	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	8 39
18	n	118/120 (98%)	100 (85%)	17 (14%)	1 (1%)	16 51
19	o	114/116 (98%)	109 (96%)	5 (4%)	0	100 100
20	p	112/114 (98%)	100 (89%)	11 (10%)	1 (1%)	14 48
21	q	115/117 (98%)	113 (98%)	2 (2%)	0	100 100
22	r	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	13 46
23	s	108/110 (98%)	99 (92%)	9 (8%)	0	100 100
24	t	91/93 (98%)	84 (92%)	7 (8%)	0	100 100
25	u	100/102 (98%)	79 (79%)	20 (20%)	1 (1%)	13 46
26	v	92/94 (98%)	85 (92%)	7 (8%)	0	100 100
27	w	73/75 (97%)	59 (81%)	14 (19%)	0	100 100
28	x	75/77 (97%)	64 (85%)	11 (15%)	0	100 100
29	y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	8 37
30	z	56/58 (97%)	55 (98%)	1 (2%)	0	100 100
31	B	54/56 (96%)	44 (82%)	9 (17%)	1 (2%)	6 34
32	C	48/50 (96%)	44 (92%)	4 (8%)	0	100 100
33	D	44/46 (96%)	40 (91%)	4 (9%)	0	100 100
34	E	62/64 (97%)	56 (90%)	6 (10%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	F	36/38 (95%)	30 (83%)	6 (17%)	0	100 100
38	G	216/225 (96%)	180 (83%)	35 (16%)	1 (0%)	25 60
39	H	204/206 (99%)	188 (92%)	16 (8%)	0	100 100
40	I	203/205 (99%)	175 (86%)	27 (13%)	1 (0%)	25 60
41	J	155/157 (99%)	115 (74%)	40 (26%)	0	100 100
42	K	98/100 (98%)	84 (86%)	14 (14%)	0	100 100
43	L	149/151 (99%)	133 (89%)	15 (10%)	1 (1%)	19 54
44	M	127/129 (98%)	118 (93%)	9 (7%)	0	100 100
45	N	125/127 (98%)	112 (90%)	13 (10%)	0	100 100
46	O	96/98 (98%)	80 (83%)	16 (17%)	0	100 100
47	P	114/116 (98%)	97 (85%)	17 (15%)	0	100 100
48	Q	121/123 (98%)	100 (83%)	19 (16%)	2 (2%)	7 36
49	R	112/114 (98%)	101 (90%)	11 (10%)	0	100 100
50	S	98/100 (98%)	86 (88%)	12 (12%)	0	100 100
51	T	86/88 (98%)	81 (94%)	3 (4%)	2 (2%)	5 31
52	U	80/82 (98%)	69 (86%)	11 (14%)	0	100 100
53	V	78/80 (98%)	64 (82%)	14 (18%)	0	100 100
54	W	63/65 (97%)	56 (89%)	6 (10%)	1 (2%)	8 37
55	X	77/79 (98%)	72 (94%)	5 (6%)	0	100 100
56	Y	83/85 (98%)	78 (94%)	5 (6%)	0	100 100
57	Z	63/65 (97%)	38 (60%)	20 (32%)	5 (8%)	1 12
All	All	6067/6690 (91%)	5327 (88%)	711 (12%)	29 (0%)	27 60

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	8	491	ARG
18	n	70	THR
11	g	9	VAL
25	u	98	ASN
38	G	18	GLN
43	L	33	GLY
57	Z	24	LYS
57	Z	37	TYR
9	e	175	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	e	176	PHE
17	m	69	PRO
17	m	70	ASP
20	p	110	LYS
29	y	24	GLU
40	I	34	GLU
51	T	44	GLU
51	T	45	HIS
8	d	86	ALA
31	B	23	ALA
48	Q	27	PRO
54	W	13	THR
57	Z	10	PRO
12	a	217	THR
57	Z	9	GLU
9	e	72	SER
22	r	54	VAL
57	Z	65	ARG
4	8	624	PRO
48	Q	3	VAL

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
4	8	236/574 (41%)	235 (100%)	1 (0%)	89 91
6	b	216/216 (100%)	211 (98%)	5 (2%)	45 64
7	c	164/164 (100%)	163 (99%)	1 (1%)	84 88
8	d	165/165 (100%)	164 (99%)	1 (1%)	84 88
9	e	148/148 (100%)	147 (99%)	1 (1%)	81 86
10	f	137/137 (100%)	134 (98%)	3 (2%)	47 65
11	g	114/114 (100%)	114 (100%)	0	100 100
12	a	110/181 (61%)	108 (98%)	2 (2%)	54 71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	i	109/110 (99%)	106 (97%)	3 (3%)	38 59
14	j	116/116 (100%)	116 (100%)	0	100 100
15	k	103/103 (100%)	100 (97%)	3 (3%)	37 59
16	l	102/102 (100%)	101 (99%)	1 (1%)	73 81
17	m	109/109 (100%)	108 (99%)	1 (1%)	75 83
18	n	100/100 (100%)	98 (98%)	2 (2%)	50 68
19	o	86/86 (100%)	83 (96%)	3 (4%)	31 54
20	p	99/99 (100%)	98 (99%)	1 (1%)	73 81
21	q	89/89 (100%)	88 (99%)	1 (1%)	70 79
22	r	84/84 (100%)	84 (100%)	0	100 100
23	s	93/93 (100%)	90 (97%)	3 (3%)	34 56
24	t	80/80 (100%)	79 (99%)	1 (1%)	65 76
25	u	83/83 (100%)	82 (99%)	1 (1%)	67 78
26	v	78/78 (100%)	76 (97%)	2 (3%)	41 61
27	w	57/57 (100%)	57 (100%)	0	100 100
28	x	67/67 (100%)	65 (97%)	2 (3%)	36 58
29	y	55/55 (100%)	55 (100%)	0	100 100
30	z	48/48 (100%)	48 (100%)	0	100 100
31	B	47/47 (100%)	46 (98%)	1 (2%)	48 67
32	C	45/45 (100%)	45 (100%)	0	100 100
33	D	38/38 (100%)	38 (100%)	0	100 100
34	E	51/51 (100%)	49 (96%)	2 (4%)	27 51
35	F	34/34 (100%)	34 (100%)	0	100 100
38	G	180/186 (97%)	178 (99%)	2 (1%)	70 79
39	H	170/170 (100%)	169 (99%)	1 (1%)	84 88
40	I	172/172 (100%)	166 (96%)	6 (4%)	31 54
41	J	119/119 (100%)	117 (98%)	2 (2%)	56 72
42	K	87/87 (100%)	85 (98%)	2 (2%)	45 64
43	L	124/124 (100%)	121 (98%)	3 (2%)	44 63
44	M	104/104 (100%)	104 (100%)	0	100 100
45	N	105/105 (100%)	104 (99%)	1 (1%)	73 81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	O	86/86 (100%)	84 (98%)	2 (2%)	45 64
47	P	89/89 (100%)	87 (98%)	2 (2%)	47 65
48	Q	103/103 (100%)	98 (95%)	5 (5%)	21 46
49	R	92/92 (100%)	92 (100%)	0	100 100
50	S	83/83 (100%)	83 (100%)	0	100 100
51	T	76/76 (100%)	74 (97%)	2 (3%)	41 61
52	U	65/65 (100%)	65 (100%)	0	100 100
53	V	74/74 (100%)	74 (100%)	0	100 100
54	W	56/56 (100%)	55 (98%)	1 (2%)	54 71
55	X	70/70 (100%)	70 (100%)	0	100 100
56	Y	65/65 (100%)	64 (98%)	1 (2%)	60 74
57	Z	55/55 (100%)	53 (96%)	2 (4%)	30 54
All	All	5038/5454 (92%)	4965 (99%)	73 (1%)	62 75

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	8	477	PHE
6	b	50	THR
6	b	52	HIS
6	b	77	VAL
6	b	172	THR
6	b	212	TRP
7	c	151	THR
8	d	84	THR
9	e	173	ASP
10	f	19	ASN
10	f	42	VAL
10	f	103	ASN
12	a	53	ARG
12	a	210	LYS
13	i	66	PHE
13	i	112	LYS
13	i	133	ARG
15	k	22	ILE
15	k	49	ARG
15	k	56	ASP
16	l	77	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	m	54	THR
18	n	56	LYS
18	n	90	ARG
19	o	3	LYS
19	o	10	ARG
19	o	69	ASP
20	p	105	LYS
21	q	5	ARG
23	s	11	ARG
23	s	77	ASP
23	s	109	ASP
24	t	80	TRP
25	u	101	THR
26	v	20	LEU
26	v	31	TYR
28	x	45	PHE
28	x	71	ARG
31	B	53	VAL
34	E	15	LYS
34	E	46	LYS
38	G	150	ILE
38	G	166	ASP
39	H	48	LYS
40	I	4	LEU
40	I	69	ARG
40	I	74	TYR
40	I	153	ARG
40	I	158	LEU
40	I	162	GLU
41	J	28	ARG
41	J	53	ARG
42	K	38	ARG
42	K	85	ILE
43	L	4	ARG
43	L	112	ASP
43	L	132	THR
45	N	90	ASP
46	O	56	HIS
46	O	89	ARG
47	P	45	THR
47	P	124	LYS
48	Q	17	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	Q	39	THR
48	Q	62	VAL
48	Q	66	ILE
48	Q	96	THR
51	T	42	PHE
51	T	53	ARG
54	W	11	ARG
56	Y	48	LYS
57	Z	32	ARG
57	Z	46	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
4	8	496	GLN
4	8	514	GLN
4	8	560	GLN
6	b	85	ASN
6	b	89	ASN
6	b	116	GLN
6	b	142	ASN
6	b	242	HIS
7	c	49	GLN
7	c	58	ASN
7	c	130	GLN
8	d	9	GLN
8	d	94	GLN
8	d	163	ASN
9	e	126	ASN
11	g	28	ASN
11	g	43	ASN
12	a	24	ASN
12	a	57	GLN
12	a	58	ASN
13	i	93	ASN
13	i	110	GLN
18	n	16	HIS
19	o	38	GLN
19	o	43	ASN
19	o	98	GLN
20	p	6	GLN
20	p	11	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	q	71	ASN
23	s	7	HIS
24	t	48	GLN
25	u	68	ASN
25	u	73	ASN
26	v	80	HIS
27	w	8	ASN
28	x	16	ASN
31	B	5	ASN
31	B	18	HIS
31	B	41	HIS
32	C	44	GLN
33	D	13	ASN
35	F	35	GLN
38	G	50	ASN
39	H	139	ASN
40	I	35	GLN
40	I	58	GLN
40	I	70	GLN
40	I	88	ASN
41	J	134	ASN
42	K	11	HIS
42	K	37	HIS
43	L	67	ASN
43	L	85	GLN
44	M	66	GLN
45	N	30	ASN
45	N	80	HIS
46	O	58	ASN
47	P	27	ASN
47	P	28	ASN
47	P	39	ASN
47	P	80	ASN
48	Q	111	GLN
50	S	65	GLN
51	T	34	GLN
52	U	26	ASN
53	V	30	HIS
54	W	53	GLN
55	X	42	ASN
56	Y	54	GLN
56	Y	67	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	Y	74	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	1538/1539 (99%)	296 (19%)	5 (0%)
2	1	2902/2903 (99%)	570 (19%)	8 (0%)
3	2	119/120 (99%)	17 (14%)	0
36	4	19/39 (48%)	6 (31%)	1 (5%)
37	5	76/77 (98%)	16 (21%)	0
5	6	76/77 (98%)	17 (22%)	0
All	All	4730/4755 (99%)	922 (19%)	14 (0%)

All (922) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	4	U
1	3	7	A
1	3	9	G
1	3	16	A
1	3	21	G
1	3	22	G
1	3	32	A
1	3	39	G
1	3	47	C
1	3	48	C
1	3	49	U
1	3	51	A
1	3	58	C
1	3	66	A
1	3	82	G
1	3	83	C
1	3	84	U
1	3	85	U
1	3	89	U
1	3	95	C
1	3	109	A
1	3	115	G
1	3	121	U
1	3	127	G
1	3	130	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	131	A
1	3	164	G
1	3	182	A
1	3	183	C
1	3	191	G
1	3	209	U
1	3	210	C
1	3	224	U
1	3	225	C
1	3	239	U
1	3	240	G
1	3	245	U
1	3	247	G
1	3	249	U
1	3	251	G
1	3	265	G
1	3	266	G
1	3	267	C
1	3	269	C
1	3	279	A
1	3	281	G
1	3	289	G
1	3	298	A
1	3	321	A
1	3	328	C
1	3	329	A
1	3	330	C
1	3	340	U
1	3	345	C
1	3	351	G
1	3	352	C
1	3	354	G
1	3	363	A
1	3	367	U
1	3	368	U
1	3	369	G
1	3	372	C
1	3	387	U
1	3	392	C
1	3	397	A
1	3	402	G
1	3	408	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	411	A
1	3	412	A
1	3	413	G
1	3	414	A
1	3	422	C
1	3	429	U
1	3	434	U
1	3	439	U
1	3	467	U
1	3	482	A
1	3	484	G
1	3	486	U
1	3	490	C
1	3	497	G
1	3	499	A
1	3	509	A
1	3	518	C
1	3	521	G
1	3	532	A
1	3	533	A
1	3	534	U
1	3	545	C
1	3	547	A
1	3	562	U
1	3	571	U
1	3	572	A
1	3	573	A
1	3	575	G
1	3	576	C
1	3	577	G
1	3	607	A
1	3	615	G
1	3	618	C
1	3	623	C
1	3	626	G
1	3	633	G
1	3	639	G
1	3	653	U
1	3	657	U
1	3	660	C
1	3	665	A
1	3	688	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	691	G
1	3	693	G
1	3	694	A
1	3	702	A
1	3	703	G
1	3	717	U
1	3	718	A
1	3	723	U
1	3	724	G
1	3	734	G
1	3	747	A
1	3	748	G
1	3	755	G
1	3	768	A
1	3	777	A
1	3	781	A
1	3	793	U
1	3	794	A
1	3	801	U
1	3	814	A
1	3	815	A
1	3	817	C
1	3	818	G
1	3	819	A
1	3	821	G
1	3	832	G
1	3	842	U
1	3	843	U
1	3	844	G
1	3	846	G
1	3	859	G
1	3	865	A
1	3	872	A
1	3	873	A
1	3	887	G
1	3	890	G
1	3	913	A
1	3	916	U
1	3	927	G
1	3	934	C
1	3	938	A
1	3	949	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	955	U
1	3	958	A
1	3	960	U
1	3	961	U
1	3	965	U
1	3	966	G
1	3	968	A
1	3	969	A
1	3	971	G
1	3	973	G
1	3	975	A
1	3	976	G
1	3	977	A
1	3	978	A
1	3	979	C
1	3	989	U
1	3	992	U
1	3	993	G
1	3	994	A
1	3	1004	A
1	3	1012	A
1	3	1015	G
1	3	1028	C
1	3	1033	G
1	3	1035	A
1	3	1036	A
1	3	1037	C
1	3	1044	A
1	3	1053	G
1	3	1054	C
1	3	1058	G
1	3	1065	U
1	3	1070	U
1	3	1074	G
1	3	1080	A
1	3	1081	A
1	3	1085	U
1	3	1091	U
1	3	1092	A
1	3	1094	G
1	3	1095	U
1	3	1101	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	1111	A
1	3	1115	U
1	3	1118	U
1	3	1124	G
1	3	1130	A
1	3	1136	C
1	3	1137	C
1	3	1138	G
1	3	1139	G
1	3	1149	C
1	3	1157	A
1	3	1158	C
1	3	1159	U
1	3	1165	U
1	3	1168	U
1	3	1169	A
1	3	1173	U
1	3	1174	G
1	3	1179	A
1	3	1181	G
1	3	1182	G
1	3	1183	U
1	3	1185	G
1	3	1191	A
1	3	1193	G
1	3	1196	A
1	3	1197	A
1	3	1200	C
1	3	1201	A
1	3	1207	G
1	3	1213	A
1	3	1221	G
1	3	1222	G
1	3	1224	U
1	3	1225	A
1	3	1226	C
1	3	1227	A
1	3	1229	A
1	3	1236	A
1	3	1238	A
1	3	1241	G
1	3	1256	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	1257	A
1	3	1275	A
1	3	1278	G
1	3	1280	A
1	3	1281	C
1	3	1282	C
1	3	1286	U
1	3	1287	A
1	3	1290	G
1	3	1291	U
1	3	1300	G
1	3	1301	U
1	3	1307	U
1	3	1308	U
1	3	1309	G
1	3	1317	C
1	3	1318	A
1	3	1320	C
1	3	1322	C
1	3	1323	G
1	3	1338	G
1	3	1346	A
1	3	1347	G
1	3	1350	A
1	3	1353	G
1	3	1363	A
1	3	1378	C
1	3	1381	U
1	3	1382	C
1	3	1385	G
1	3	1389	C
1	3	1394	A
1	3	1395	C
1	3	1397	C
1	3	1399	C
1	3	1400	C
1	3	1401	G
1	3	1411	C
1	3	1429	A
1	3	1433	A
1	3	1446	A
1	3	1448	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3	1451	U
1	3	1452	C
1	3	1491	G
1	3	1492	A
1	3	1493	A
1	3	1494	G
1	3	1497	G
1	3	1503	A
1	3	1504	G
1	3	1505	G
1	3	1513	A
1	3	1517	G
1	3	1520	C
1	3	1522	U
1	3	1525	G
1	3	1528	U
1	3	1529	G
1	3	1530	G
1	3	1533	C
2	1	8	C
2	1	10	A
2	1	12	U
2	1	23	G
2	1	34	U
2	1	46	G
2	1	49	A
2	1	50	U
2	1	51	G
2	1	56	A
2	1	60	G
2	1	63	A
2	1	71	A
2	1	74	A
2	1	75	G
2	1	84	A
2	1	86	G
2	1	88	G
2	1	92	U
2	1	110	G
2	1	116	C
2	1	117	G
2	1	119	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	120	U
2	1	121	G
2	1	125	A
2	1	126	A
2	1	138	U
2	1	140	C
2	1	141	G
2	1	142	A
2	1	143	C
2	1	149	A
2	1	162	U
2	1	163	C
2	1	177	G
2	1	181	A
2	1	196	A
2	1	200	U
2	1	201	C
2	1	204	A
2	1	216	A
2	1	221	A
2	1	222	A
2	1	229	C
2	1	233	A
2	1	241	A
2	1	248	G
2	1	255	A
2	1	264	C
2	1	266	G
2	1	276	U
2	1	281	C
2	1	294	A
2	1	310	A
2	1	323	C
2	1	324	A
2	1	329	G
2	1	330	A
2	1	333	G
2	1	345	A
2	1	346	A
2	1	353	C
2	1	371	A
2	1	372	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	380	G
2	1	386	G
2	1	387	U
2	1	389	G
2	1	395	U
2	1	396	G
2	1	397	U
2	1	404	A
2	1	406	G
2	1	411	G
2	1	412	A
2	1	424	G
2	1	435	C
2	1	446	G
2	1	451	U
2	1	456	C
2	1	457	A
2	1	479	A
2	1	480	A
2	1	481	G
2	1	491	G
2	1	501	A
2	1	502	A
2	1	504	A
2	1	505	A
2	1	508	A
2	1	509	C
2	1	510	C
2	1	512	G
2	1	521	U
2	1	529	A
2	1	531	C
2	1	532	A
2	1	544	C
2	1	548	G
2	1	549	G
2	1	550	C
2	1	560	C
2	1	563	A
2	1	572	A
2	1	575	A
2	1	589	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	603	A
2	1	614	A
2	1	615	U
2	1	616	A
2	1	627	A
2	1	628	G
2	1	632	A
2	1	637	A
2	1	645	C
2	1	646	U
2	1	648	G
2	1	655	A
2	1	659	G
2	1	664	G
2	1	685	A
2	1	686	U
2	1	696	G
2	1	711	G
2	1	714	U
2	1	729	G
2	1	730	A
2	1	747	C
2	1	748	G
2	1	752	A
2	1	753	A
2	1	762	U
2	1	764	A
2	1	765	C
2	1	775	G
2	1	776	G
2	1	782	A
2	1	783	A
2	1	784	G
2	1	785	G
2	1	789	A
2	1	793	A
2	1	800	A
2	1	804	A
2	1	805	G
2	1	811	U
2	1	812	C
2	1	819	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	827	U
2	1	829	A
2	1	831	G
2	1	845	A
2	1	846	U
2	1	847	U
2	1	859	G
2	1	871	U
2	1	872	U
2	1	873	C
2	1	874	G
2	1	878	A
2	1	883	G
2	1	885	C
2	1	886	A
2	1	887	U
2	1	891	G
2	1	897	C
2	1	898	C
2	1	910	A
2	1	912	C
2	1	913	U
2	1	914	G
2	1	915	C
2	1	931	U
2	1	932	U
2	1	941	A
2	1	945	A
2	1	946	C
2	1	959	A
2	1	961	C
2	1	962	G
2	1	965	C
2	1	974	G
2	1	975	A
2	1	983	A
2	1	985	C
2	1	990	A
2	1	995	C
2	1	1004	U
2	1	1012	U
2	1	1013	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	1026	G
2	1	1033	U
2	1	1045	C
2	1	1046	A
2	1	1047	G
2	1	1050	A
2	1	1053	C
2	1	1061	U
2	1	1065	U
2	1	1066	U
2	1	1067	A
2	1	1068	G
2	1	1069	A
2	1	1070	A
2	1	1071	G
2	1	1072	C
2	1	1076	C
2	1	1078	U
2	1	1083	U
2	1	1088	A
2	1	1089	A
2	1	1090	A
2	1	1094	U
2	1	1097	U
2	1	1104	C
2	1	1111	A
2	1	1126	A
2	1	1130	U
2	1	1131	G
2	1	1132	U
2	1	1133	A
2	1	1135	C
2	1	1142	A
2	1	1157	G
2	1	1169	A
2	1	1170	C
2	1	1173	U
2	1	1174	U
2	1	1175	A
2	1	1176	U
2	1	1177	G
2	1	1178	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	1180	U
2	1	1181	U
2	1	1204	A
2	1	1205	A
2	1	1206	G
2	1	1212	G
2	1	1221	C
2	1	1247	A
2	1	1248	G
2	1	1250	G
2	1	1251	C
2	1	1252	G
2	1	1253	A
2	1	1255	U
2	1	1256	G
2	1	1265	A
2	1	1267	U
2	1	1268	A
2	1	1269	A
2	1	1271	G
2	1	1272	A
2	1	1280	G
2	1	1284	A
2	1	1285	A
2	1	1286	A
2	1	1289	C
2	1	1296	G
2	1	1300	G
2	1	1301	A
2	1	1303	G
2	1	1313	U
2	1	1314	C
2	1	1326	U
2	1	1329	U
2	1	1341	G
2	1	1345	C
2	1	1365	A
2	1	1367	A
2	1	1378	A
2	1	1379	U
2	1	1383	A
2	1	1394	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	1396	U
2	1	1403	A
2	1	1416	G
2	1	1419	A
2	1	1420	A
2	1	1428	C
2	1	1429	G
2	1	1443	U
2	1	1453	A
2	1	1454	C
2	1	1461	C
2	1	1468	U
2	1	1475	G
2	1	1482	G
2	1	1488	C
2	1	1490	A
2	1	1491	G
2	1	1493	C
2	1	1498	C
2	1	1503	A
2	1	1515	A
2	1	1522	A
2	1	1523	U
2	1	1529	G
2	1	1535	A
2	1	1536	C
2	1	1537	G
2	1	1542	U
2	1	1547	C
2	1	1552	A
2	1	1553	A
2	1	1563	U
2	1	1567	G
2	1	1569	A
2	1	1572	A
2	1	1583	A
2	1	1584	U
2	1	1585	C
2	1	1593	A
2	1	1599	U
2	1	1603	A
2	1	1608	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	1610	A
2	1	1616	A
2	1	1617	C
2	1	1618	A
2	1	1627	G
2	1	1635	A
2	1	1647	U
2	1	1648	U
2	1	1649	G
2	1	1653	G
2	1	1654	A
2	1	1657	U
2	1	1662	U
2	1	1665	A
2	1	1674	G
2	1	1698	A
2	1	1699	G
2	1	1700	A
2	1	1703	G
2	1	1715	G
2	1	1729	U
2	1	1730	C
2	1	1731	G
2	1	1732	C
2	1	1733	G
2	1	1758	U
2	1	1759	A
2	1	1764	C
2	1	1766	G
2	1	1772	A
2	1	1773	A
2	1	1782	U
2	1	1784	A
2	1	1786	A
2	1	1800	C
2	1	1801	A
2	1	1802	A
2	1	1808	A
2	1	1809	A
2	1	1810	A
2	1	1811	G
2	1	1813	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	1816	C
2	1	1819	A
2	1	1829	A
2	1	1833	C
2	1	1834	U
2	1	1838	C
2	1	1851	U
2	1	1882	U
2	1	1891	G
2	1	1896	G
2	1	1901	A
2	1	1906	G
2	1	1912	A
2	1	1913	A
2	1	1914	C
2	1	1915	U
2	1	1918	A
2	1	1919	A
2	1	1930	G
2	1	1935	G
2	1	1937	A
2	1	1939	U
2	1	1940	U
2	1	1945	G
2	1	1947	C
2	1	1955	U
2	1	1963	U
2	1	1964	G
2	1	1967	C
2	1	1969	A
2	1	1970	A
2	1	1971	U
2	1	1972	G
2	1	1978	A
2	1	1982	U
2	1	1987	A
2	1	1991	U
2	1	1993	U
2	1	1997	C
2	1	2002	G
2	1	2020	A
2	1	2022	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	2023	C
2	1	2030	A
2	1	2031	A
2	1	2032	G
2	1	2034	U
2	1	2035	G
2	1	2036	C
2	1	2043	C
2	1	2046	G
2	1	2049	G
2	1	2055	C
2	1	2056	G
2	1	2060	A
2	1	2061	G
2	1	2062	A
2	1	2063	C
2	1	2069	G
2	1	2072	C
2	1	2095	A
2	1	2100	G
2	1	2110	G
2	1	2111	U
2	1	2112	G
2	1	2115	G
2	1	2118	U
2	1	2119	A
2	1	2126	A
2	1	2131	U
2	1	2132	U
2	1	2133	G
2	1	2134	A
2	1	2137	U
2	1	2143	C
2	1	2144	G
2	1	2145	C
2	1	2158	A
2	1	2159	G
2	1	2162	G
2	1	2164	C
2	1	2166	U
2	1	2172	U
2	1	2173	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	2174	C
2	1	2181	U
2	1	2182	U
2	1	2186	G
2	1	2197	U
2	1	2198	A
2	1	2203	U
2	1	2204	G
2	1	2210	U
2	1	2211	A
2	1	2212	A
2	1	2213	U
2	1	2225	A
2	1	2238	G
2	1	2251	G
2	1	2252	G
2	1	2253	G
2	1	2258	C
2	1	2259	U
2	1	2268	A
2	1	2269	G
2	1	2279	G
2	1	2283	C
2	1	2287	A
2	1	2288	A
2	1	2300	C
2	1	2305	U
2	1	2309	A
2	1	2310	C
2	1	2325	G
2	1	2327	A
2	1	2333	A
2	1	2347	C
2	1	2382	G
2	1	2383	G
2	1	2385	C
2	1	2390	U
2	1	2391	G
2	1	2406	A
2	1	2417	C
2	1	2422	C
2	1	2423	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	2425	A
2	1	2427	C
2	1	2428	G
2	1	2429	G
2	1	2434	A
2	1	2436	G
2	1	2441	U
2	1	2444	G
2	1	2445	G
2	1	2448	A
2	1	2476	A
2	1	2487	G
2	1	2497	A
2	1	2498	C
2	1	2499	C
2	1	2500	U
2	1	2502	G
2	1	2504	U
2	1	2505	G
2	1	2513	A
2	1	2518	A
2	1	2520	C
2	1	2529	G
2	1	2535	G
2	1	2547	A
2	1	2549	G
2	1	2554	U
2	1	2556	C
2	1	2566	A
2	1	2567	G
2	1	2572	A
2	1	2574	G
2	1	2577	A
2	1	2602	A
2	1	2603	G
2	1	2609	U
2	1	2613	U
2	1	2621	G
2	1	2623	G
2	1	2629	U
2	1	2634	A
2	1	2645	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	2646	C
2	1	2649	C
2	1	2658	C
2	1	2681	C
2	1	2682	A
2	1	2684	U
2	1	2689	U
2	1	2690	U
2	1	2712	C
2	1	2713	U
2	1	2714	G
2	1	2727	A
2	1	2732	G
2	1	2733	A
2	1	2744	G
2	1	2748	A
2	1	2751	G
2	1	2765	A
2	1	2771	C
2	1	2778	A
2	1	2779	U
2	1	2791	G
2	1	2794	C
2	1	2797	U
2	1	2799	A
2	1	2800	A
2	1	2801	G
2	1	2808	G
2	1	2820	A
2	1	2821	A
2	1	2822	G
2	1	2833	U
2	1	2848	G
2	1	2849	U
2	1	2866	U
2	1	2867	G
2	1	2868	A
2	1	2872	A
2	1	2880	C
2	1	2884	U
2	1	2893	A
2	1	2894	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1	2899	A
3	2	15	A
3	2	16	G
3	2	24	G
3	2	35	C
3	2	36	C
3	2	37	C
3	2	40	U
3	2	41	G
3	2	42	C
3	2	44	G
3	2	70	C
3	2	88	C
3	2	89	U
3	2	90	C
3	2	97	C
3	2	105	G
3	2	109	A
5	6	4	G
5	6	7	G
5	6	8	U
5	6	9	G
5	6	10	G
5	6	14	A
5	6	16	C
5	6	17(A)	U
5	6	19	G
5	6	20	U
5	6	21	A
5	6	22	G
5	6	35	A
5	6	43	A
5	6	47	U
5	6	59	A
5	6	76	A
36	4	12	A
36	4	13	A
36	4	14	A
36	4	15	A
36	4	16	A
36	4	24	U
37	5	2	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	5	3	G
37	5	5	G
37	5	6	A
37	5	8	U
37	5	16	C
37	5	18	G
37	5	19	G
37	5	20	U
37	5	21	A
37	5	22	G
37	5	36	G
37	5	53	G
37	5	59	A
37	5	61	C
37	5	73	A

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3	781	A
1	3	889	A
1	3	1157	A
1	3	1307	U
1	3	1397	C
2	1	784	G
2	1	871	U
2	1	873	C
2	1	896	A
2	1	961	C
2	1	1130	U
2	1	1730	C
2	1	2326	C
36	4	13	A

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

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

5.5 Carbohydrates (i)

There are no 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.

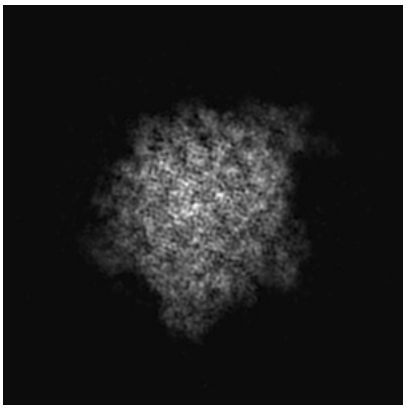
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25405. These allow visual inspection of the internal detail of the map and identification of artifacts.

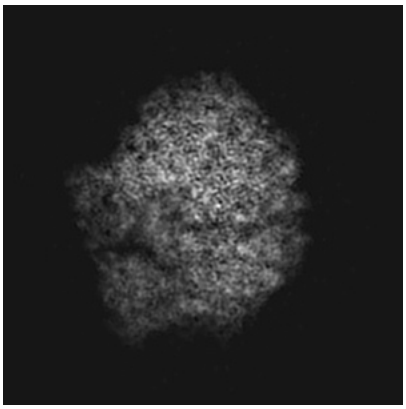
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

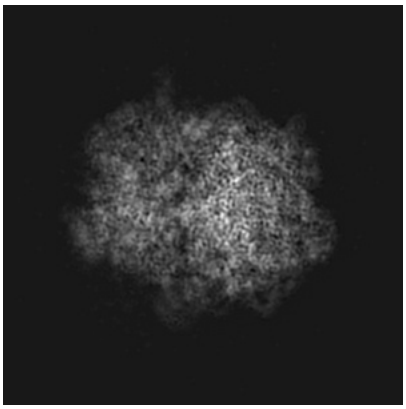
6.1.1 Primary map



X

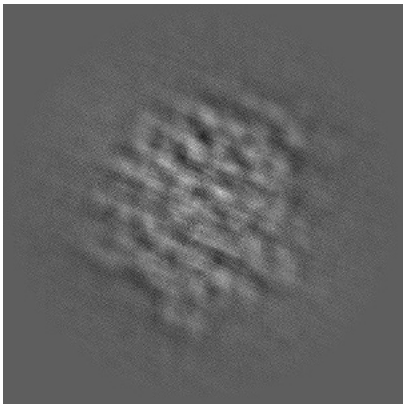


Y

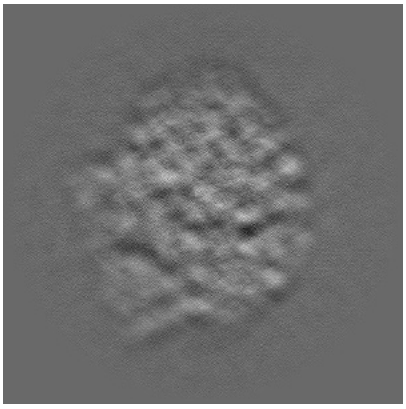


Z

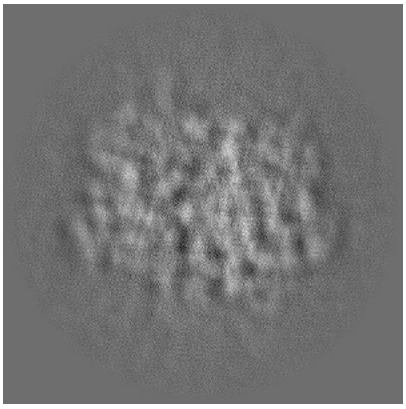
6.1.2 Raw map



X



Y

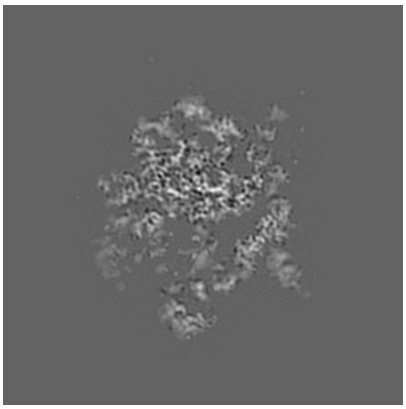


Z

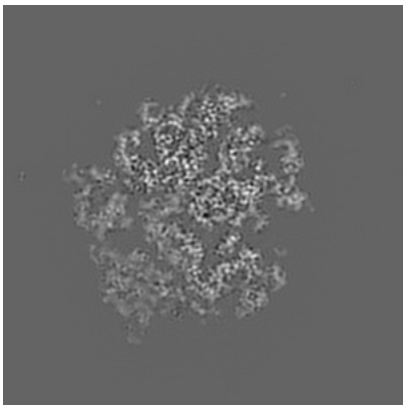
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

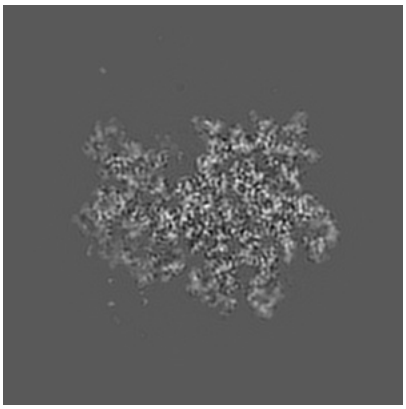
6.2.1 Primary map



X Index: 224

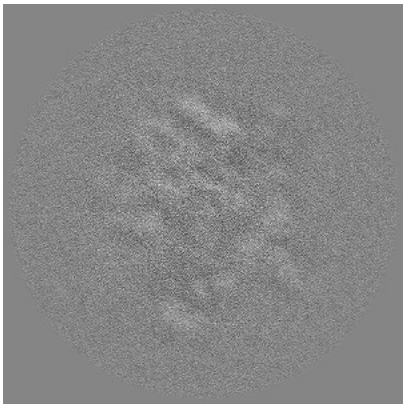


Y Index: 224

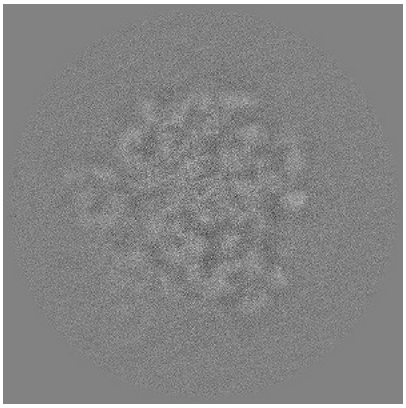


Z Index: 224

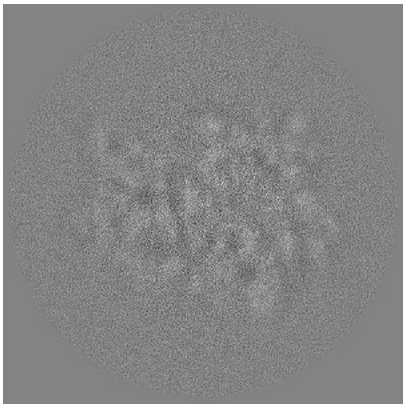
6.2.2 Raw map



X Index: 224



Y Index: 224

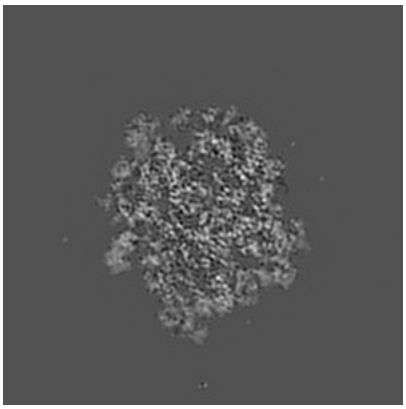


Z Index: 224

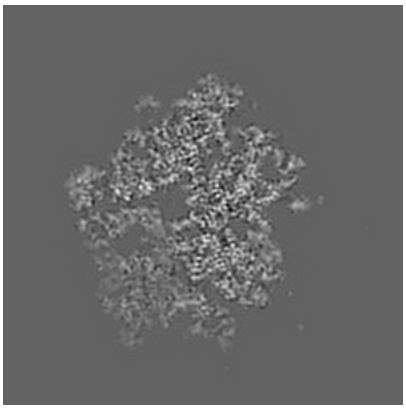
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

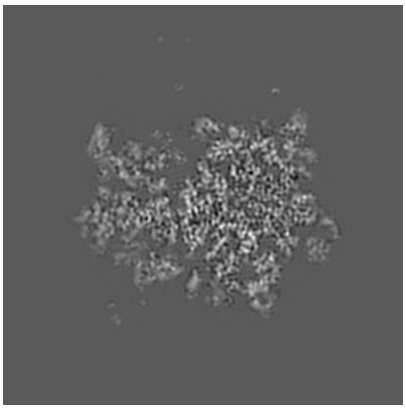
6.3.1 Primary map



X Index: 255

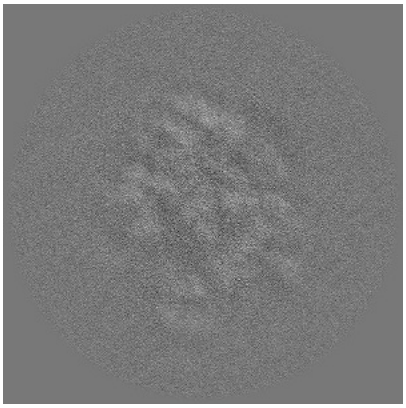


Y Index: 209

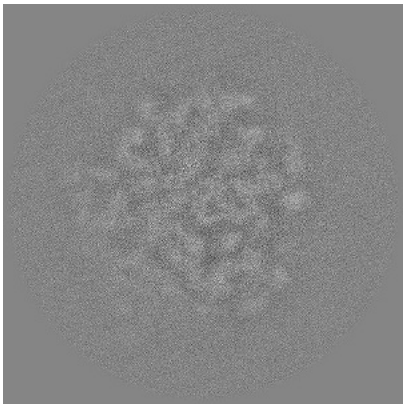


Z Index: 220

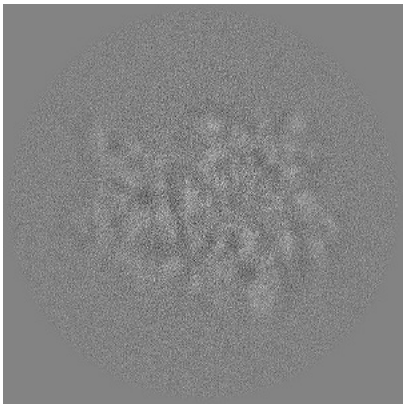
6.3.2 Raw map



X Index: 230



Y Index: 223

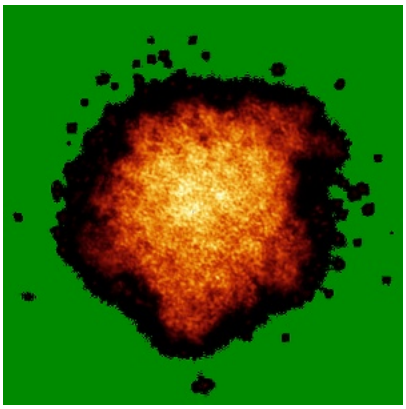


Z Index: 224

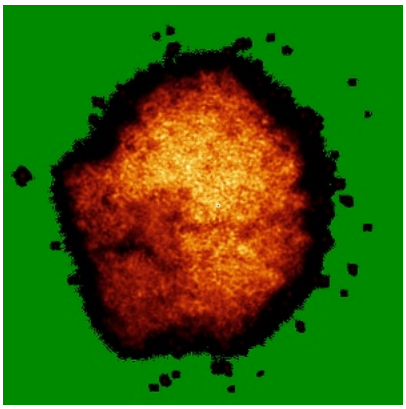
The images above show the largest variance slices of the map in three orthogonal directions.

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

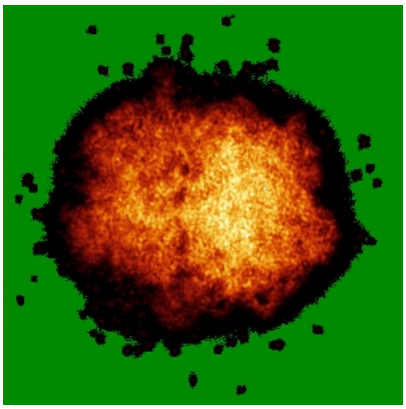
6.4.1 Primary map



X

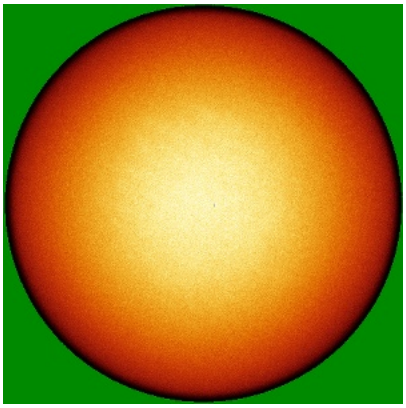


Y

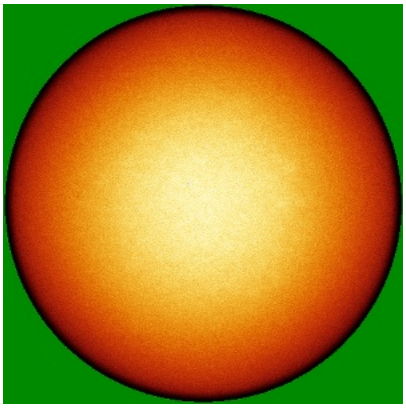


Z

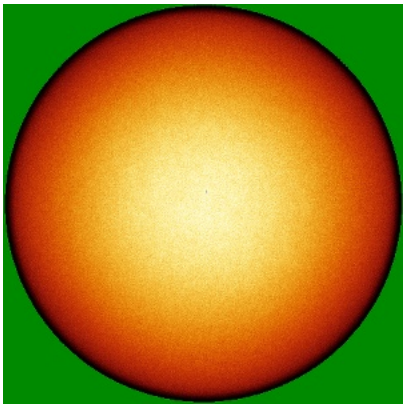
6.4.2 Raw map



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.

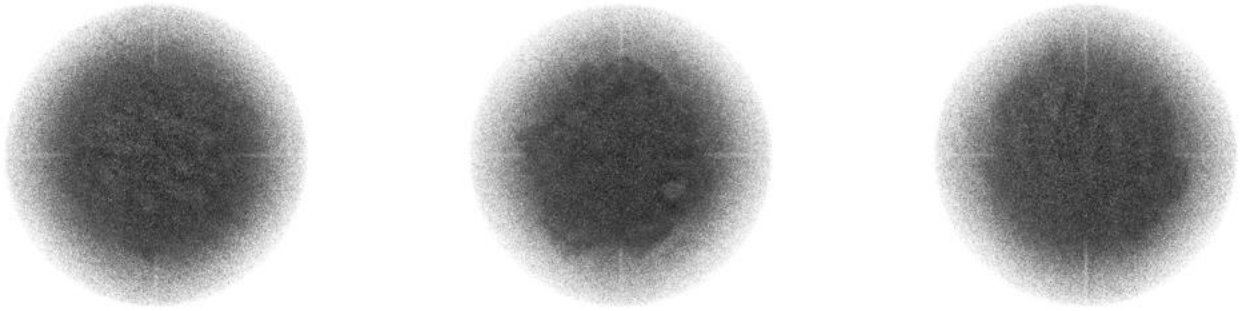
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 1.75. 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.

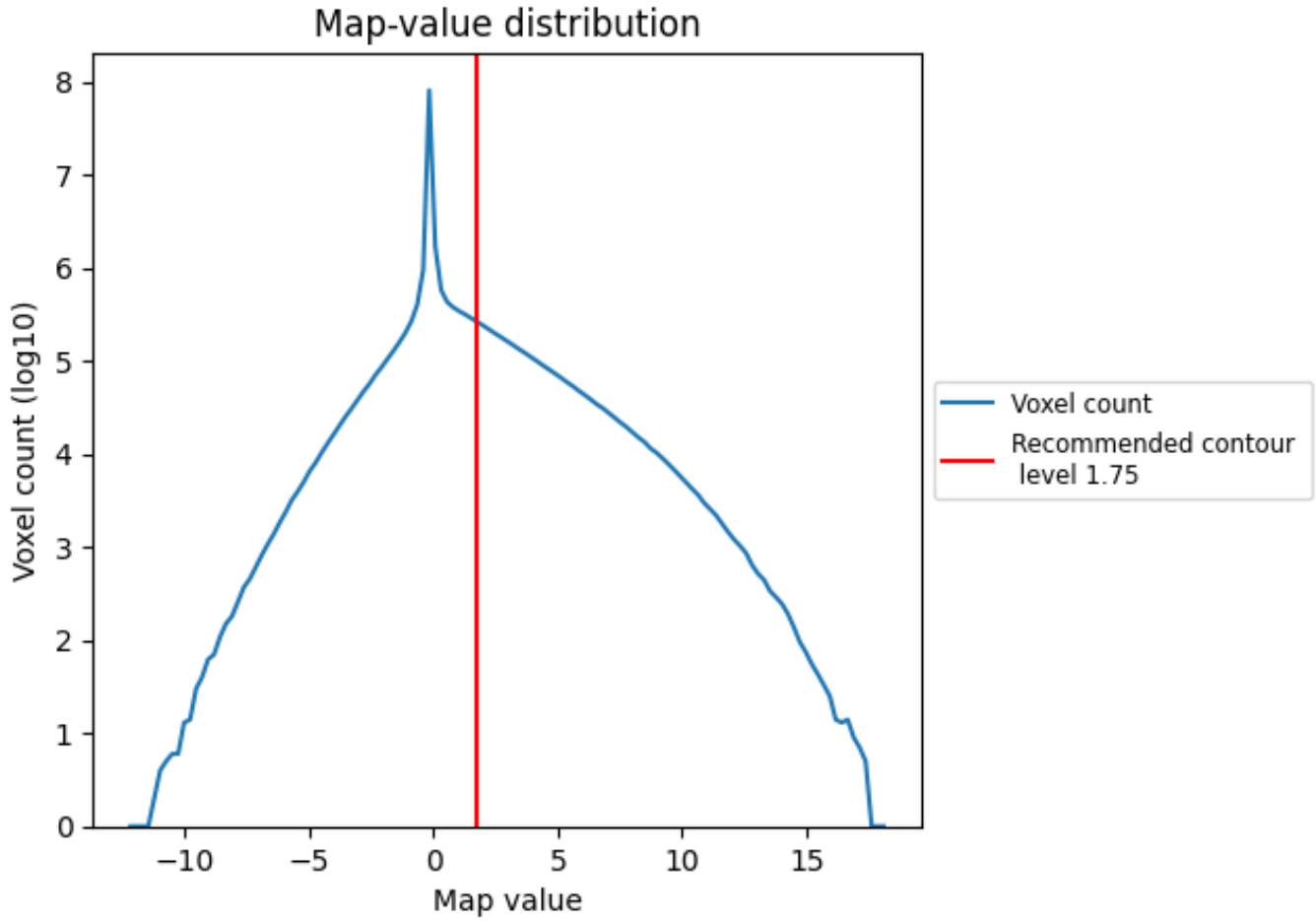
6.6 Mask visualisation (i)

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

7 Map analysis

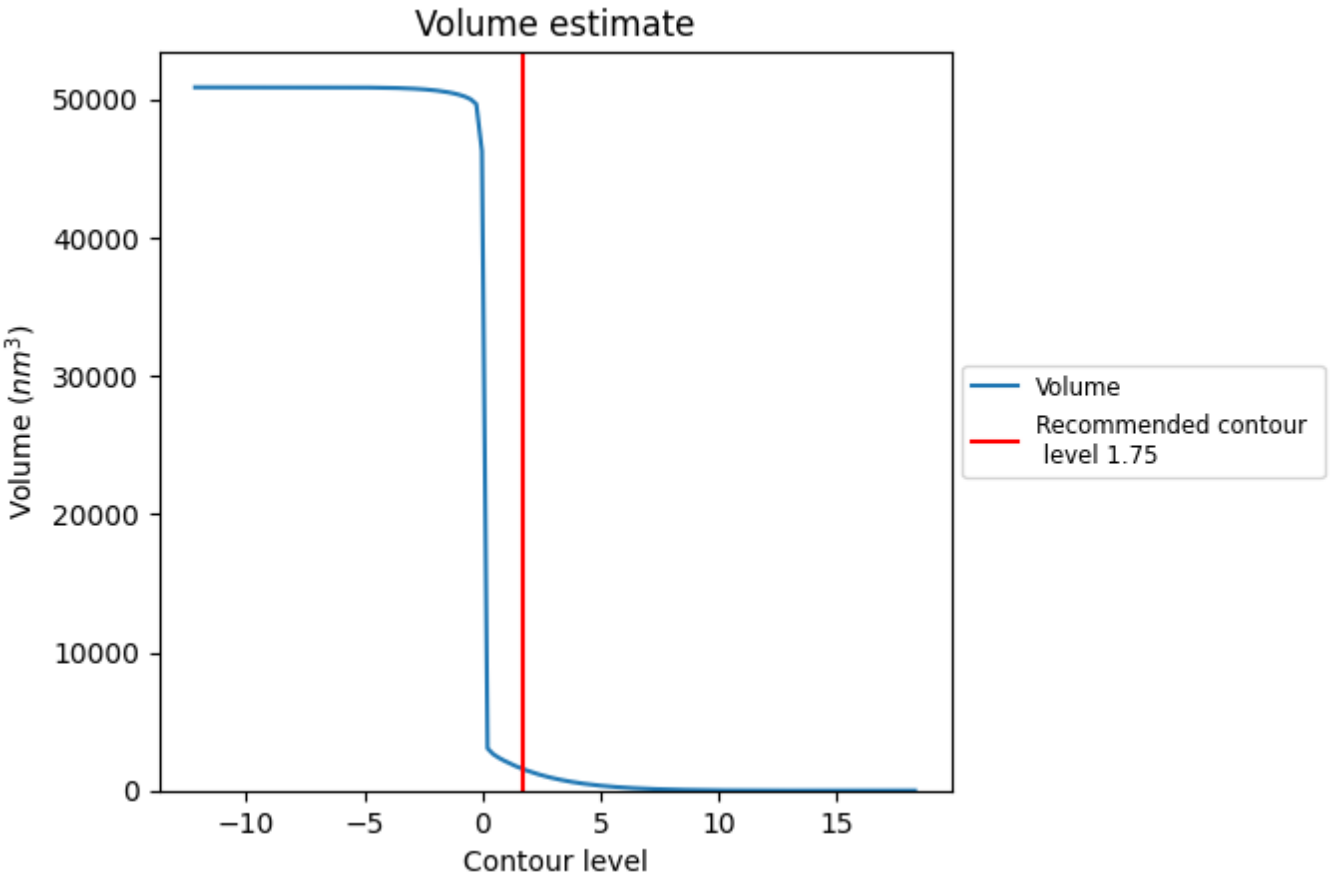
This section contains the results of statistical analysis of the map.

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.

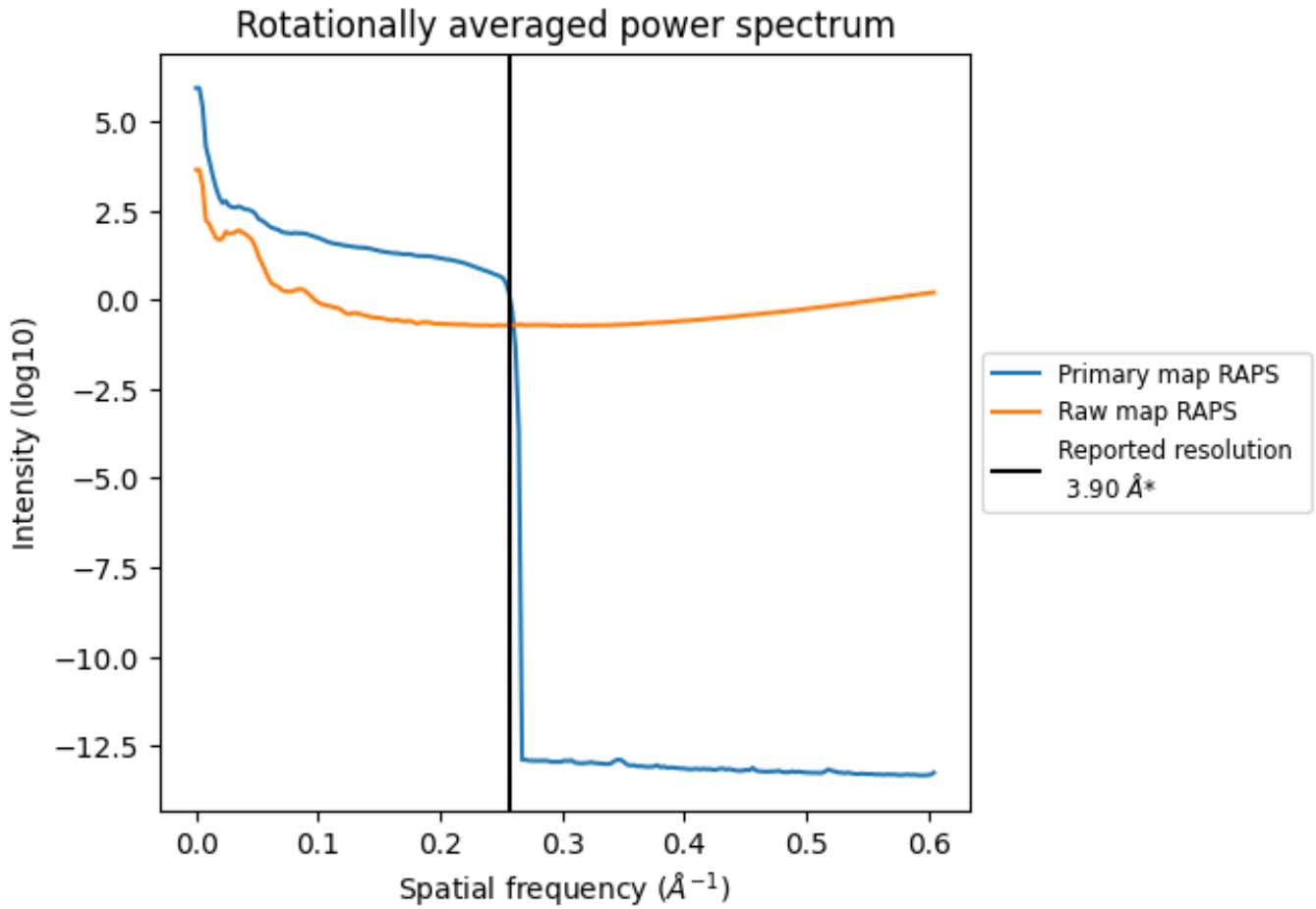
7.2 Volume estimate



The volume at the recommended contour level is 1540 nm^3; this corresponds to an approximate mass of 1391 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)

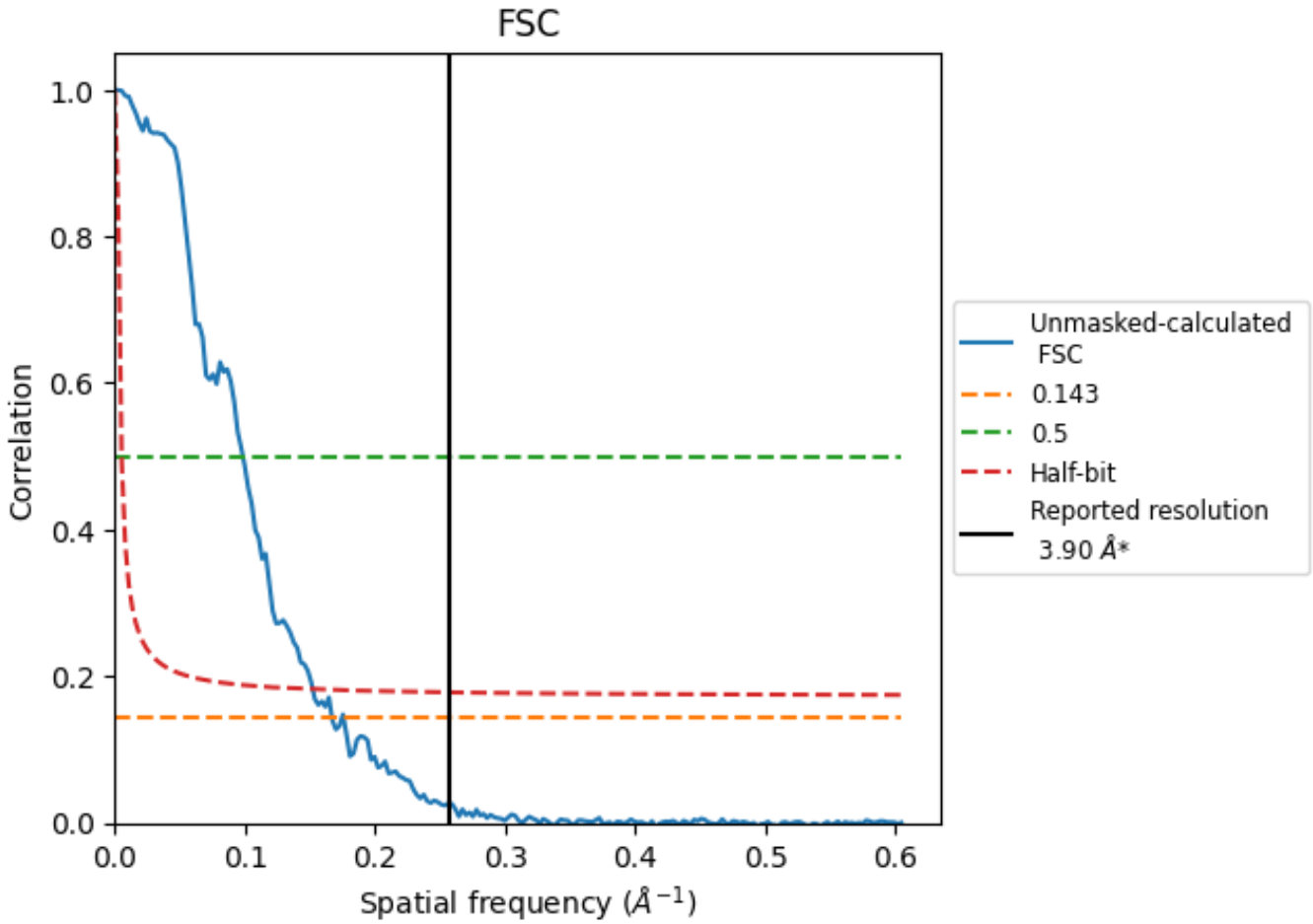


*Reported resolution corresponds to spatial frequency of 0.256 $Å^{-1}$

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

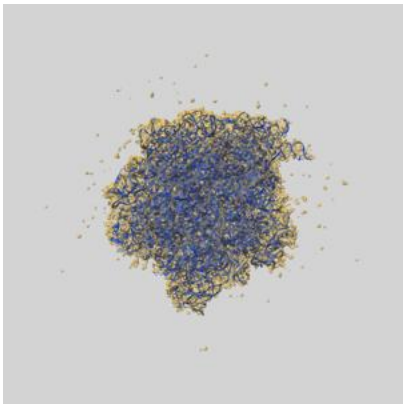
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.99	10.16	6.57

*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 5.99 differs from the reported value 3.9 by more than 10 %

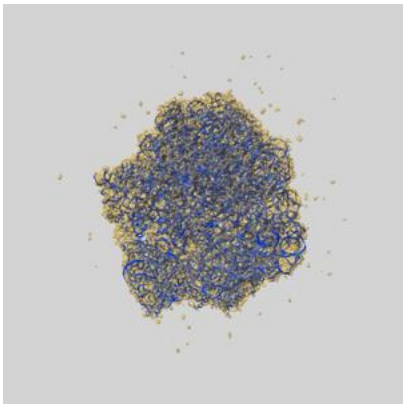
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25405 and PDB model 7SS9. Per-residue inclusion information can be found in section 3 on page 14.

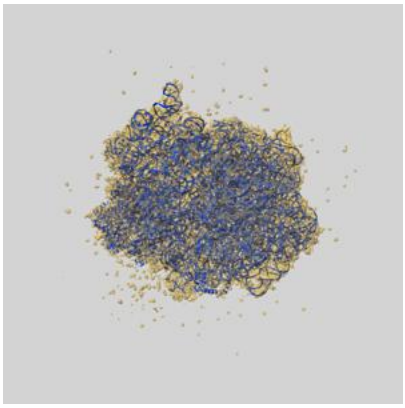
9.1 Map-model overlay



X



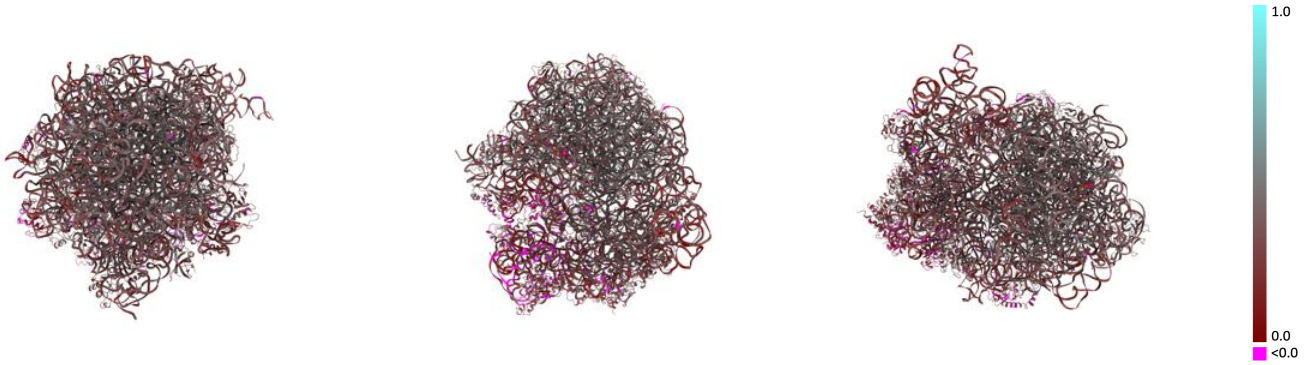
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.75 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.

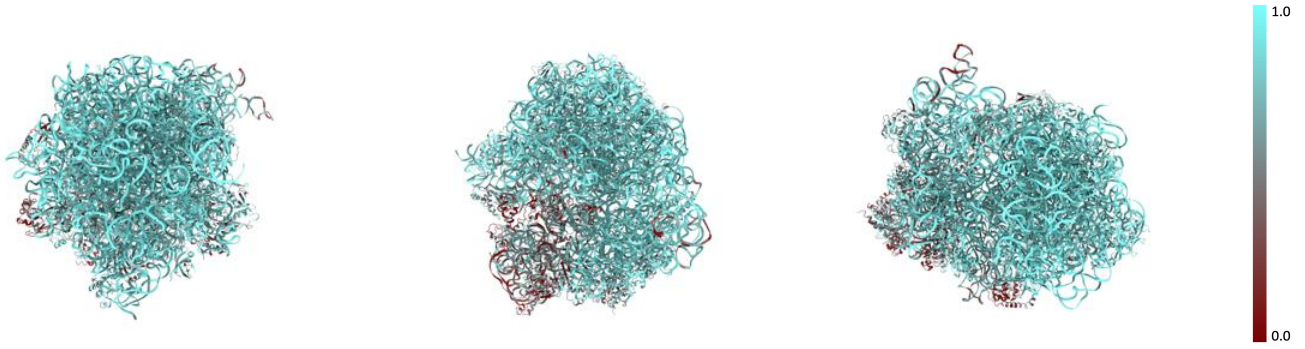
9.2 Q-score mapped to coordinate model (i)



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.

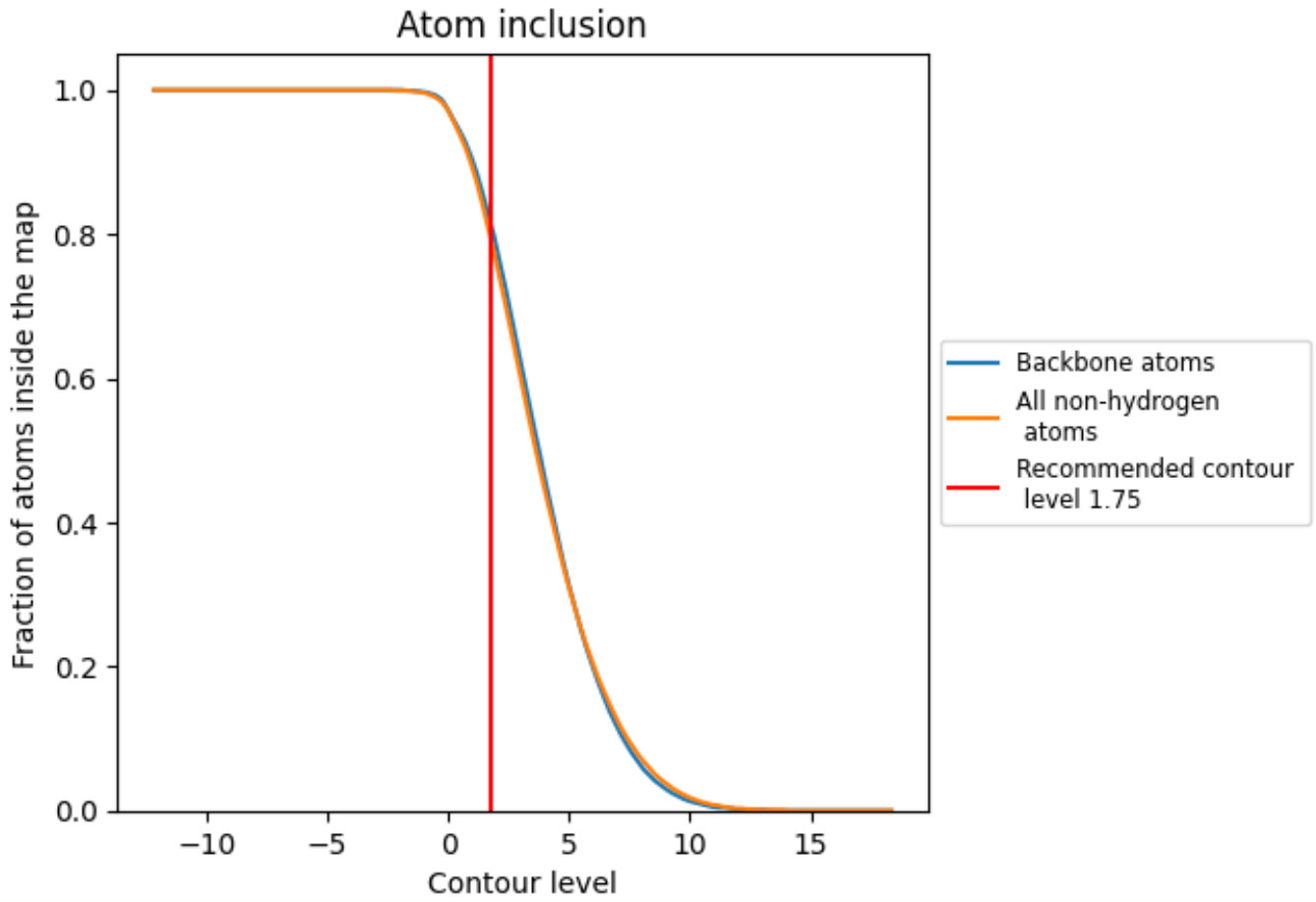
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.75).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 80% 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 (1.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7950	0.3080
1	0.9080	0.3500
2	0.8900	0.3120
3	0.7730	0.2510
4	0.4930	0.1330
5	0.7160	0.1690
6	0.4670	0.1300
8	0.4500	0.2220
B	0.8320	0.3680
C	0.6220	0.3180
D	0.8820	0.4190
E	0.8620	0.4320
F	0.7470	0.3670
G	0.5660	0.2790
H	0.3830	0.2000
I	0.6960	0.2720
J	0.7640	0.3480
K	0.7990	0.3140
L	0.2180	0.1360
M	0.8000	0.3380
N	0.3760	0.1750
O	0.3730	0.2200
P	0.7710	0.3210
Q	0.7880	0.3170
R	0.2920	0.1480
S	0.4930	0.1790
T	0.7870	0.3150
U	0.7240	0.3160
V	0.7440	0.3070
W	0.7280	0.3140
X	0.4690	0.1930
Y	0.7610	0.3070
Z	0.6450	0.2800
a	0.1850	0.1220
b	0.8560	0.4090

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	0.8260	0.4000
d	0.7720	0.3560
e	0.7000	0.2510
f	0.7230	0.2820
g	0.4430	0.2200
i	0.2570	0.1370
j	0.8240	0.3850
k	0.8320	0.3960
l	0.7960	0.3950
m	0.8460	0.4070
n	0.8210	0.4000
o	0.7740	0.3180
p	0.8460	0.3850
q	0.8520	0.3900
r	0.7990	0.3590
s	0.8280	0.3960
t	0.7860	0.3750
u	0.7830	0.3360
v	0.7940	0.3320
w	0.8440	0.4070
x	0.8540	0.3910
y	0.7910	0.3200
z	0.7990	0.3590