



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 06:07 pm GMT

PDB ID : 5O2R  
EMDB ID : EMD-3730  
Title : Cryo-EM structure of the proline-rich antimicrobial peptide Api137 bound to the terminating ribosome  
Authors : Graf, M.; Berninghausen, O.; Beckmann, R.; Wilson, D.N.  
Deposited on : 2017-05-22  
Resolution : 3.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

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

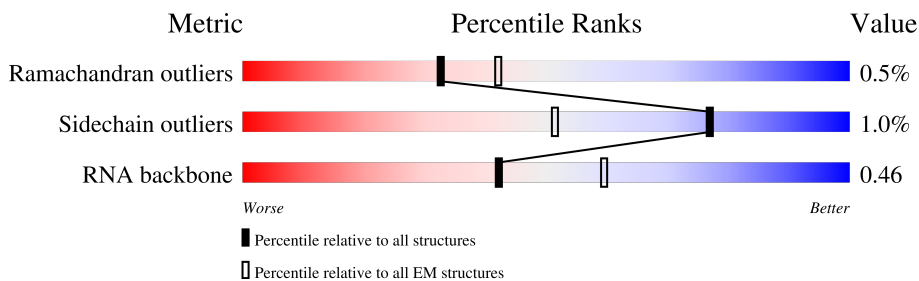
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	120	
3	C	271	
4	D	209	
5	E	201	
6	F	177	
7	G	176	
8	H	149	

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Mol	Chain	Length	Quality of chain
9	I	141	97% 99%
10	J	142	16% 100%
11	K	122	20% 99%
12	L	143	17% 98%
13	M	136	17% 98%
14	N	120	9% 99%
15	O	116	22% 100%
16	P	114	20% 98%
17	Q	117	15% 99%
18	R	103	27% 98%
19	S	110	16% 99%
20	T	93	28% 100%
21	U	102	32% 100%
22	V	94	28% 100%
23	W	75	8% 99%
24	X	77	25% 99%
25	Y	63	41% 100%
26	Z	58	10% 100%
27	0	56	18% 100%
28	1	50	38% 100%
29	2	46	9% 100%
30	3	64	6% 98%
31	4	38	16% 100%
32	5	131	98% 98%
33	6	66	61% 100%

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Mol	Chain	Length	Quality of chain
34	7	7	
35	a	1539	
36	b	218	
37	c	206	
38	d	205	
39	e	157	
40	f	100	
41	g	151	
42	h	129	
43	i	127	
44	j	98	
45	k	116	
46	l	123	
47	m	114	
48	n	101	
49	o	88	
50	p	82	
51	q	80	
52	r	65	
53	s	79	
54	t	85	
55	u	65	
56	v	242	
57	x	77	
58	z	14	

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147985 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2900	62262	27774	11460	20128	2900	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	C	U	conflict	GB 802133627
A	1847	G	A	conflict	GB 802133627

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2572	1145	471	836	120	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1150448909

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

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

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

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



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

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	50	Total	C	N	O	S	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	7	Total	C	N	O	P	0	0
			149	67	27	48	7		

- Molecule 35 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	1539	Total	C	N	O	P	0	0
			33016	14725	6052	10700	1539		

- Molecule 36 is a protein called 30S ribosomal protein S2.

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

- Molecule 37 is a protein called 30S ribosomal protein S3.

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

- Molecule 38 is a protein called 30S ribosomal protein S4.

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

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

- Molecule 40 is a protein called 30S ribosomal protein S6.

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

- Molecule 41 is a protein called 30S ribosomal protein S7.

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

- Molecule 42 is a protein called 30S ribosomal protein S8.

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

- Molecule 43 is a protein called 30S ribosomal protein S9.

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

- Molecule 44 is a protein called 30S ribosomal protein S10.

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

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	k	116	869	535	173	158	3	0	0

- Molecule 46 is a protein called 30S ribosomal protein S12.

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

- Molecule 47 is a protein called 30S ribosomal protein S13.

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

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 49 is a protein called 30S ribosomal protein S15.

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

- Molecule 50 is a protein called 30S ribosomal protein S16.

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

- Molecule 51 is a protein called 30S ribosomal protein S17.

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

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	r	65	Total	C	N	O	0	0
			504	317	96	91		

- Molecule 53 is a protein called 30S ribosomal protein S19.

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

- Molecule 54 is a protein called 30S ribosomal protein S20.

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

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 56 is a protein called Peptide chain release factor RF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	v	242	Total	C	N	O	S	0	0
			1880	1151	359	362	8		

- Molecule 57 is a RNA chain called P-site Ile-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	77	Total	C	N	O	P	0	0
			1647	734	296	540	77		

- Molecule 58 is a protein called Apidaecin.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	z	14	Total	C	N	O	0	0
			120	80	25	15		

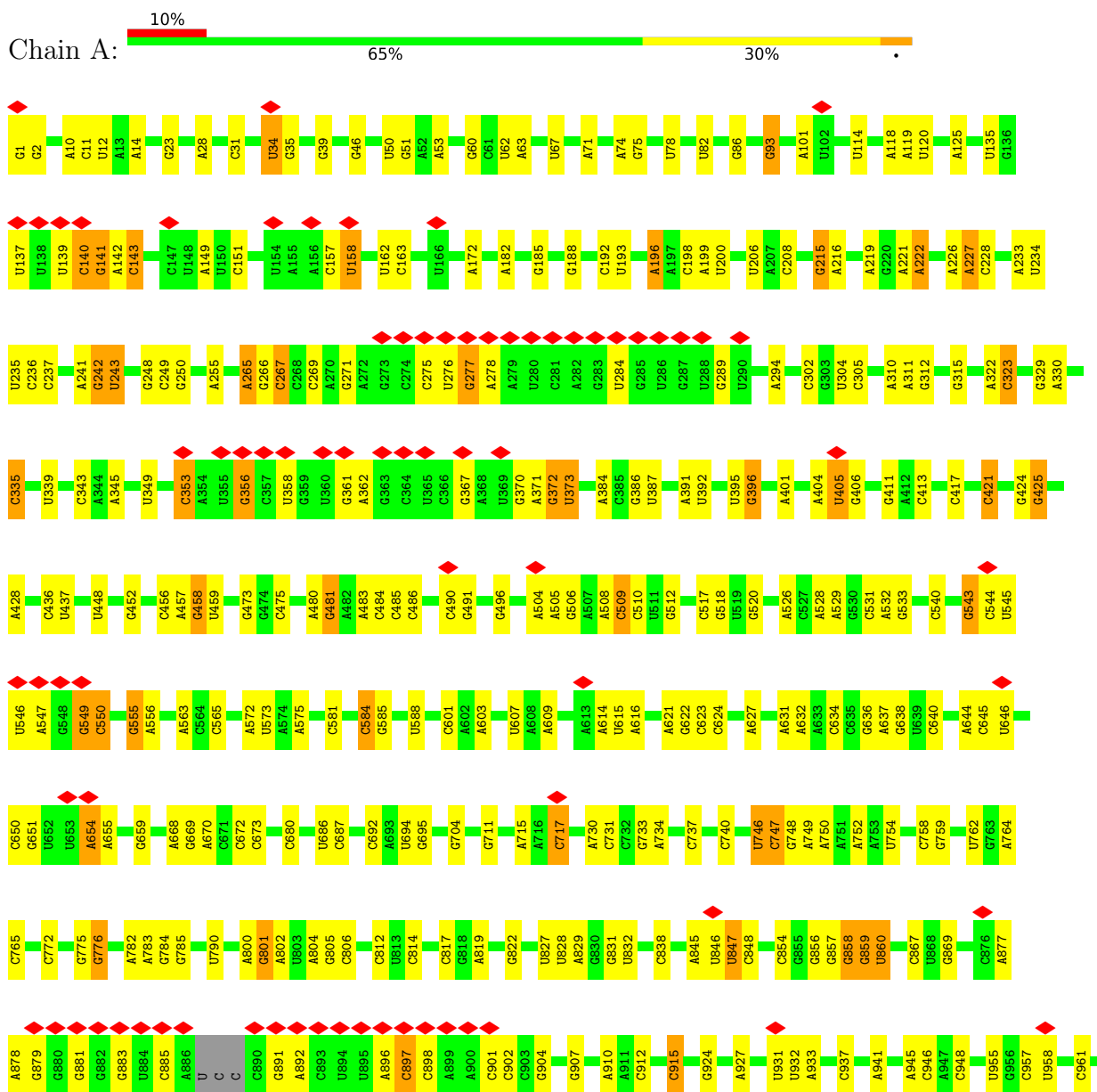
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	10	ARG	GLN	conflict	UNP Q8WSY8

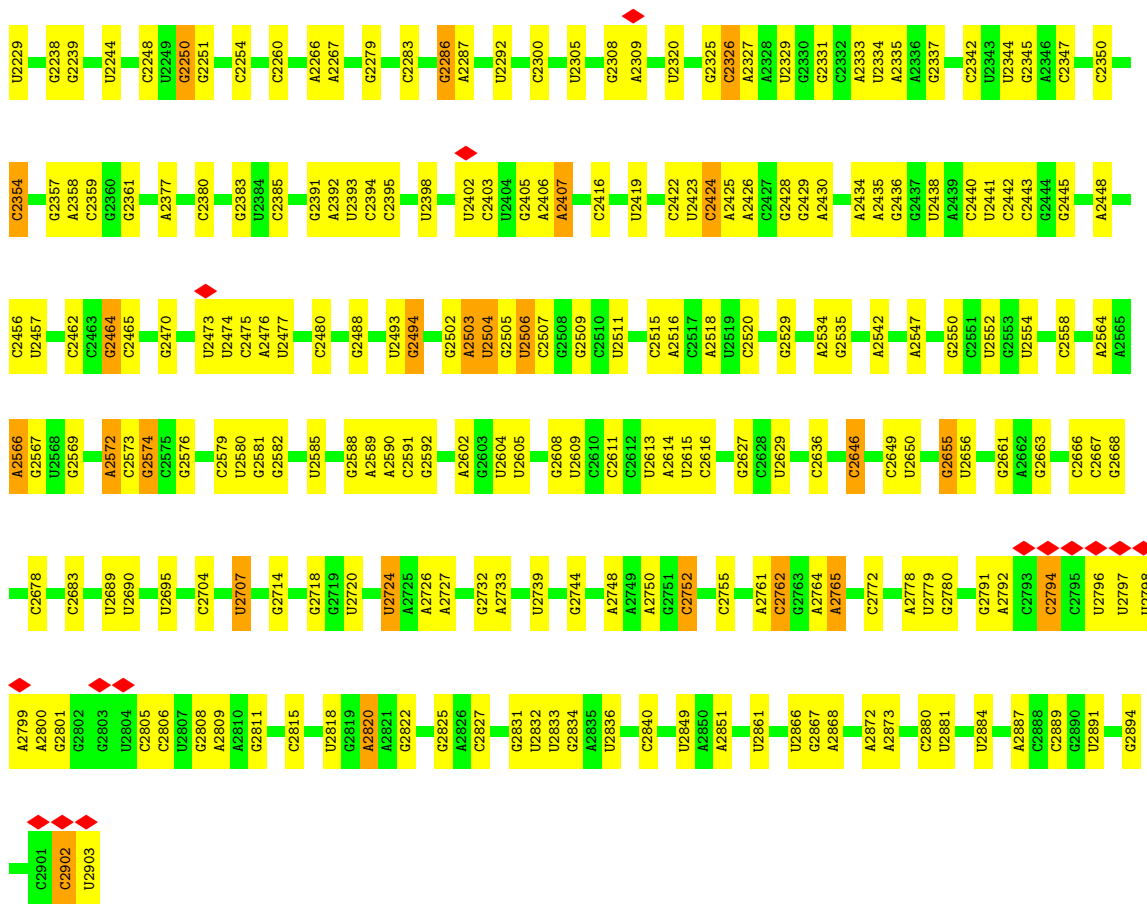
### 3 Residue-property plots [i](#)

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

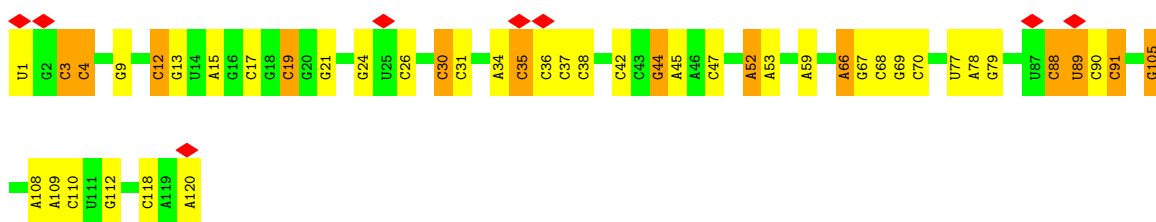
- Molecule 1: 23S ribosomal RNA



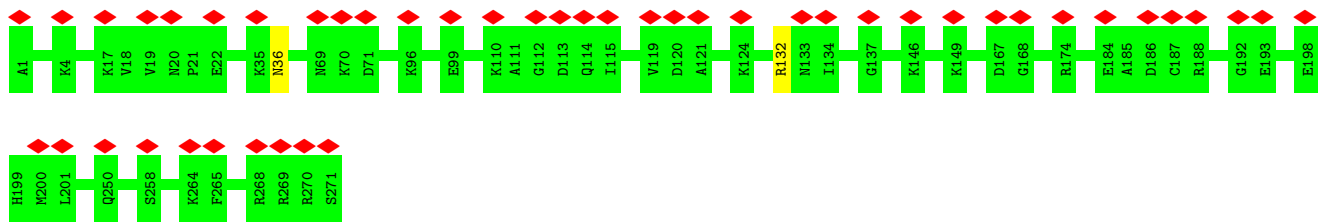




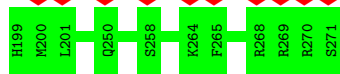
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

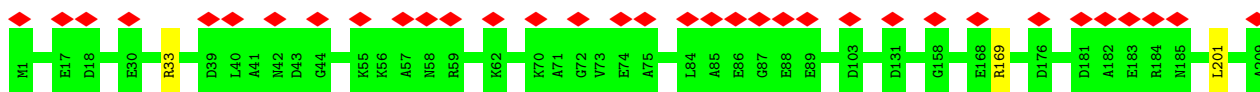


• Molecule 4: 50S ribosomal protein L3



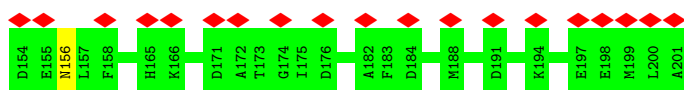
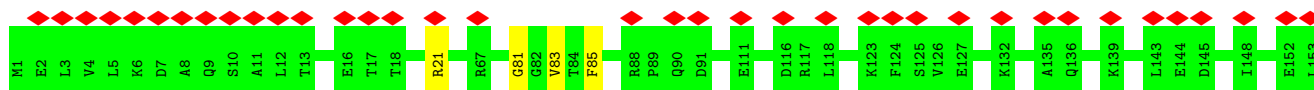


Chain D:  16% 99%



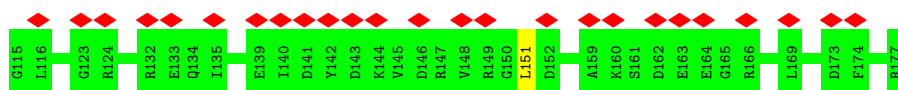
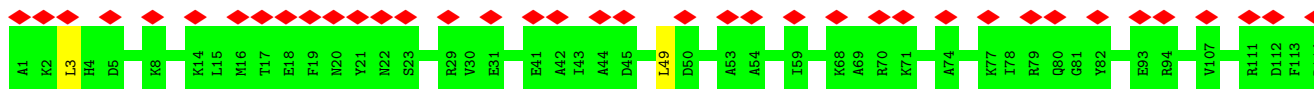
• Molecule 5: 50S ribosomal protein L4

Chain E:  28% 98%



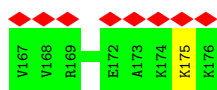
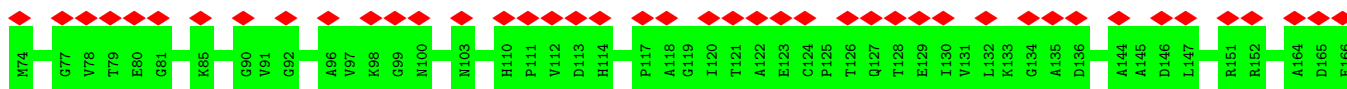
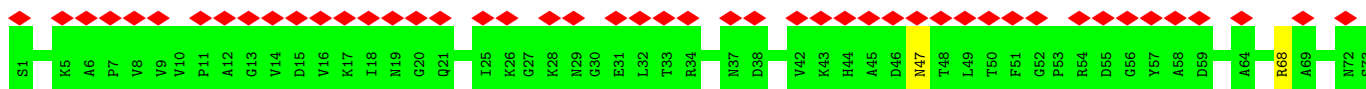
• Molecule 6: 50S ribosomal protein L5

Chain F:  36% 98%

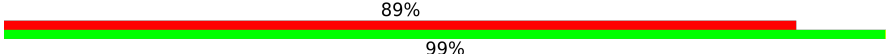


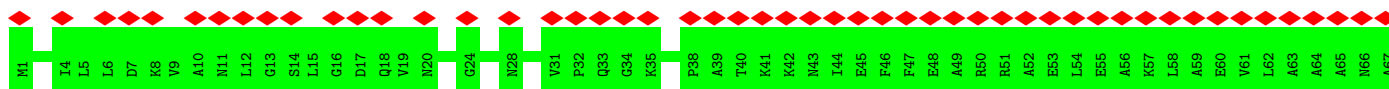
• Molecule 7: 50S ribosomal protein L6

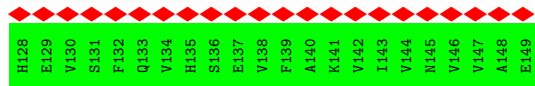
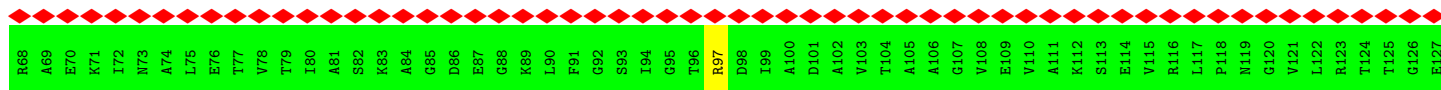
Chain G:  56% 98%



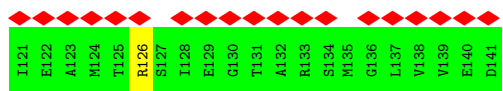
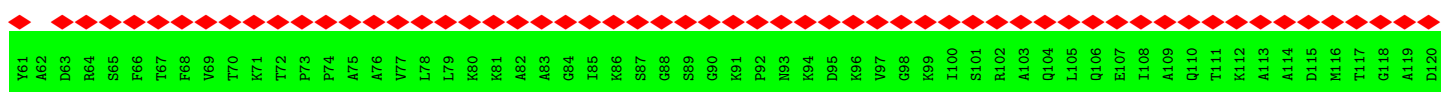
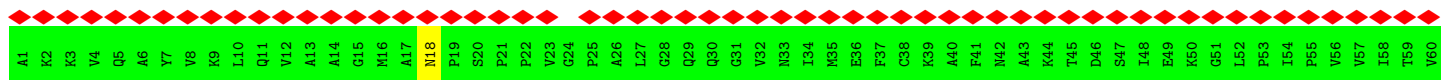
• Molecule 8: 50S ribosomal protein L9

Chain H:  89% 99%

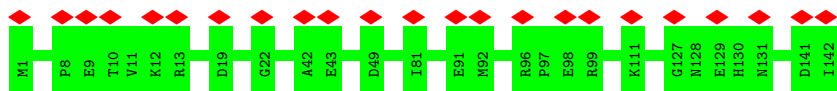




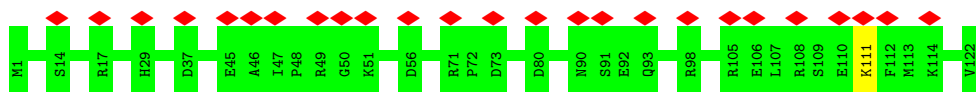
• Molecule 9: 50S ribosomal protein L11



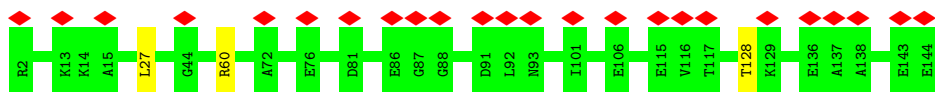
• Molecule 10: 50S ribosomal protein L13



• Molecule 11: 50S ribosomal protein L14

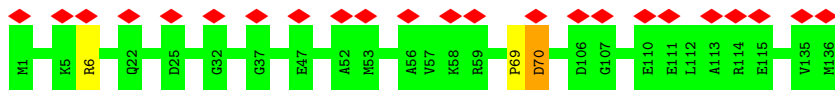


• Molecule 12: 50S ribosomal protein L15

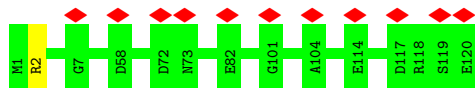


• Molecule 13: 50S ribosomal protein L16

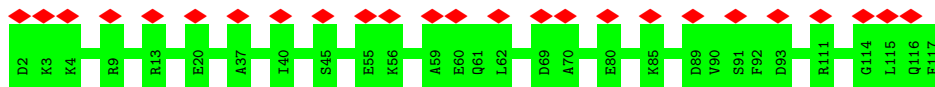




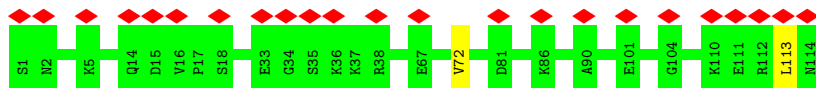
- Molecule 14: 50S ribosomal protein L17



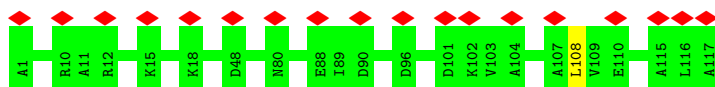
- Molecule 15: 50S ribosomal protein L18



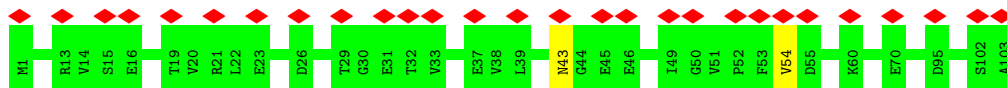
- Molecule 16: 50S ribosomal protein L19



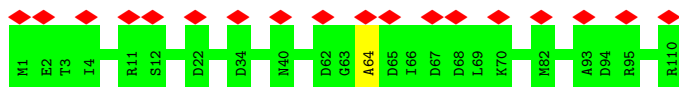
- Molecule 17: 50S ribosomal protein L20



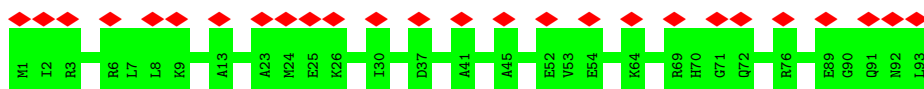
- Molecule 18: 50S ribosomal protein L21



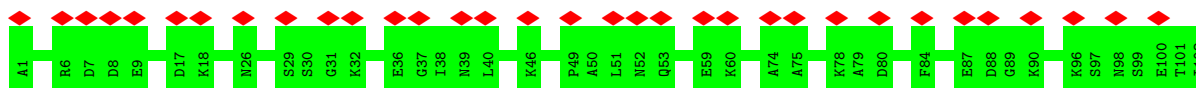
- Molecule 19: 50S ribosomal protein L22



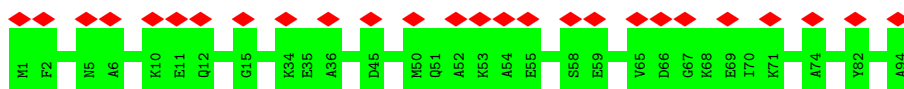
- Molecule 20: 50S ribosomal protein L23



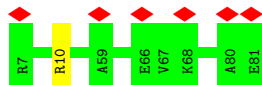
- Molecule 21: 50S ribosomal protein L24



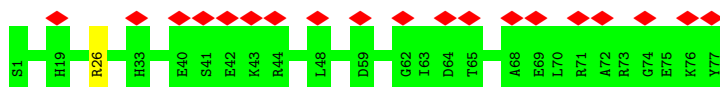
- Molecule 22: 50S ribosomal protein L25



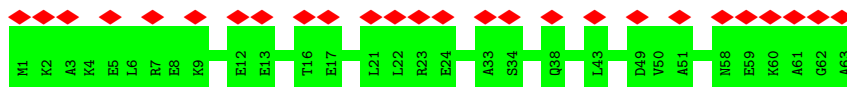
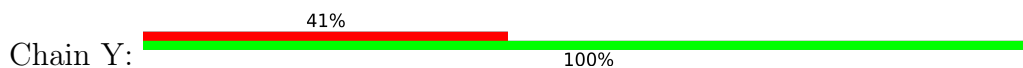
- Molecule 23: 50S ribosomal protein L27



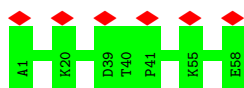
- Molecule 24: 50S ribosomal protein L28



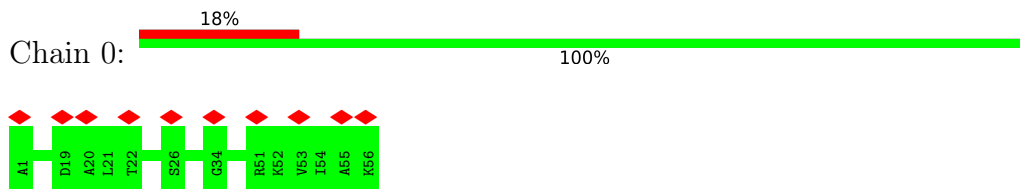
- Molecule 25: 50S ribosomal protein L29



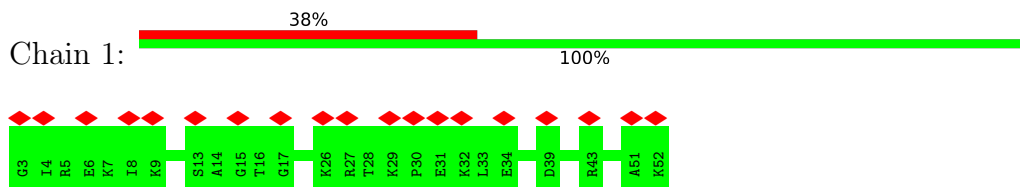
- Molecule 26: 50S ribosomal protein L30



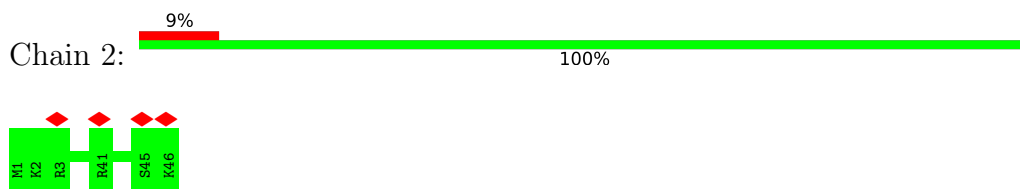
- Molecule 27: 50S ribosomal protein L32



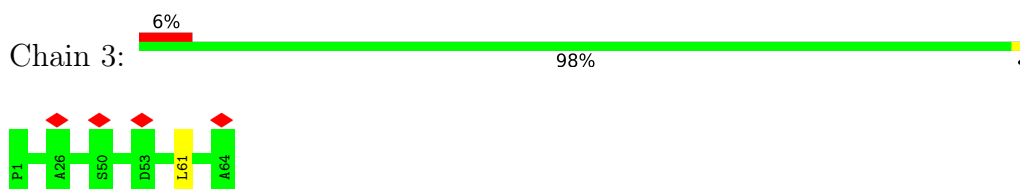
- Molecule 28: 50S ribosomal protein L33



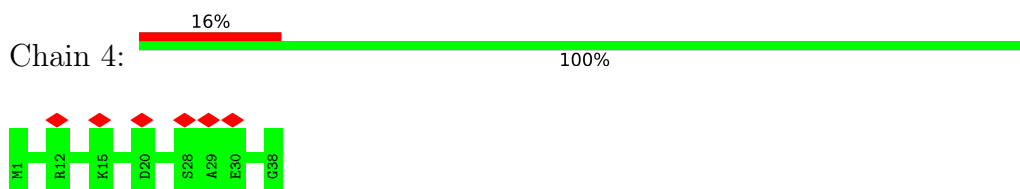
- Molecule 29: 50S ribosomal protein L34



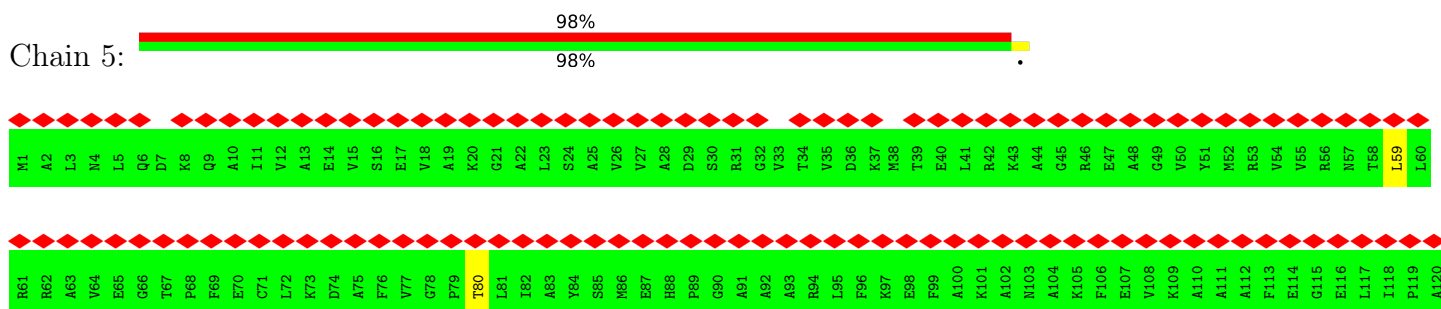
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

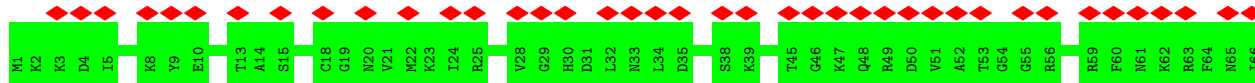


- Molecule 32: 50S ribosomal protein L10





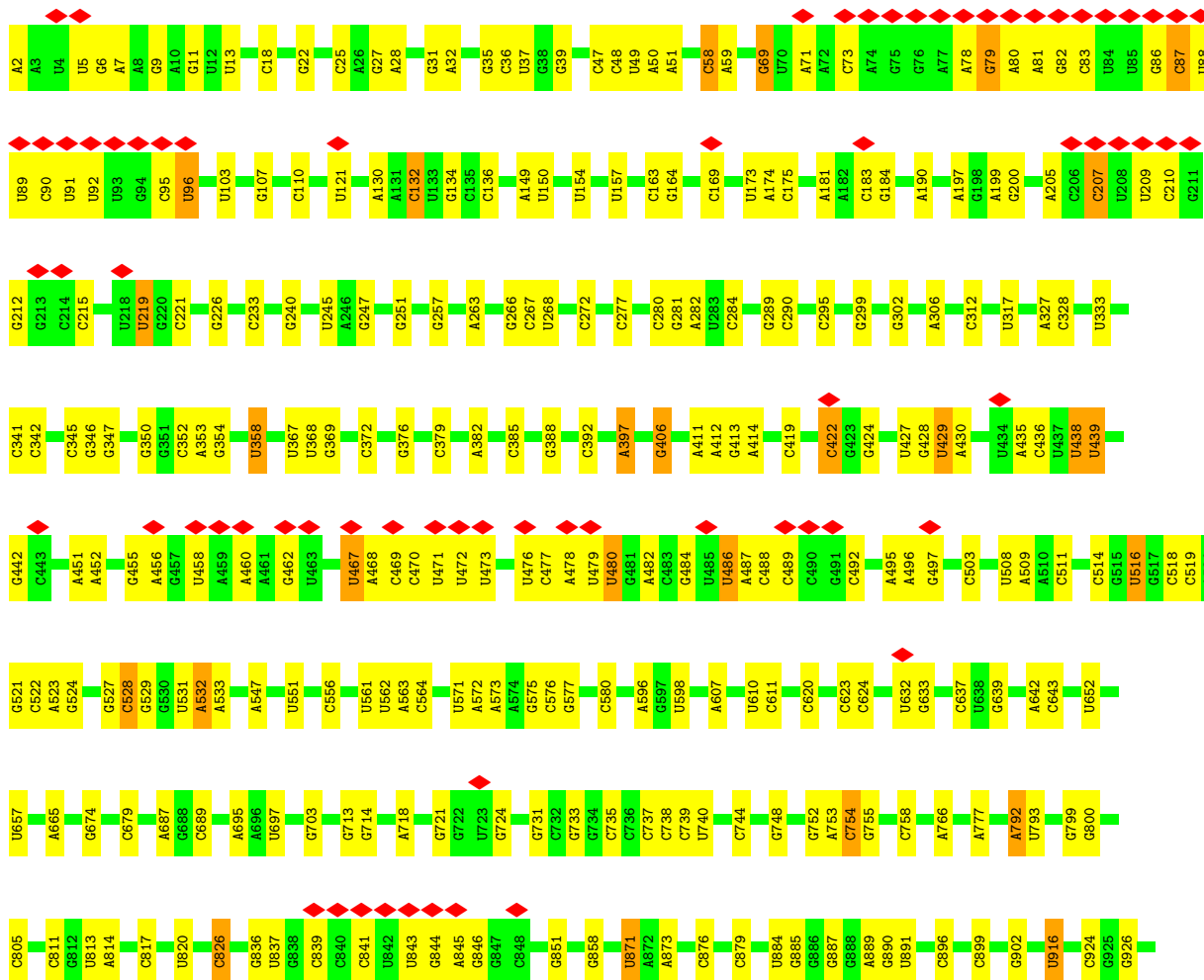
• Molecule 33: 50S ribosomal protein L31



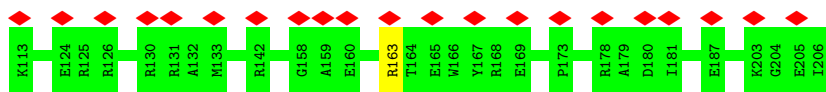
• Molecule 34: mRNA



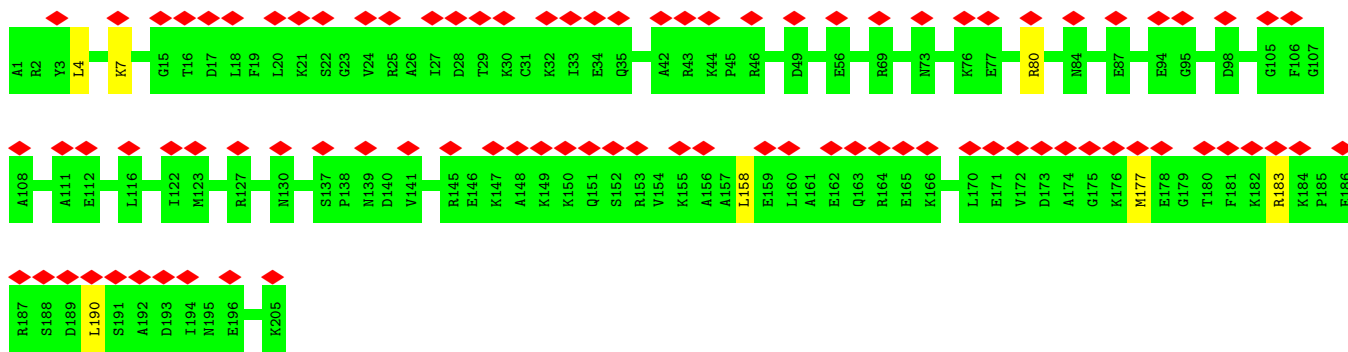
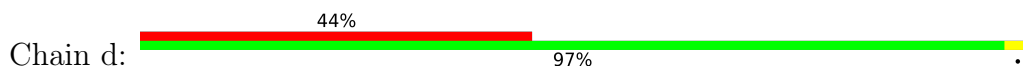
• Molecule 35: 16S ribosomal RNA



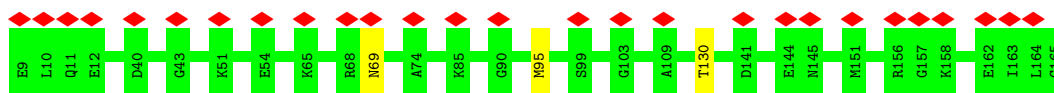




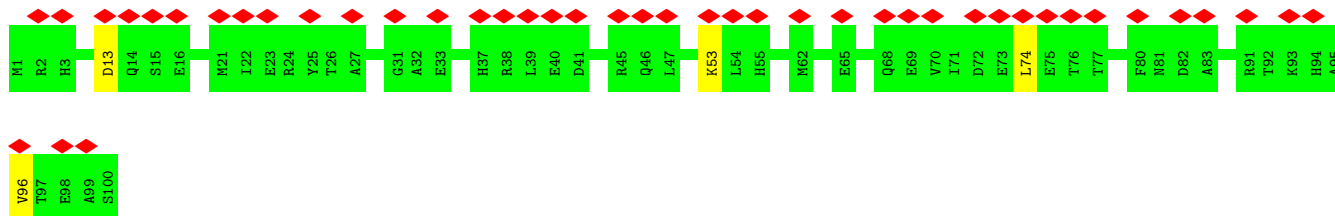
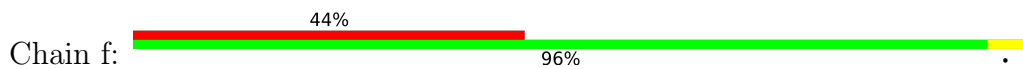
- Molecule 38: 30S ribosomal protein S4



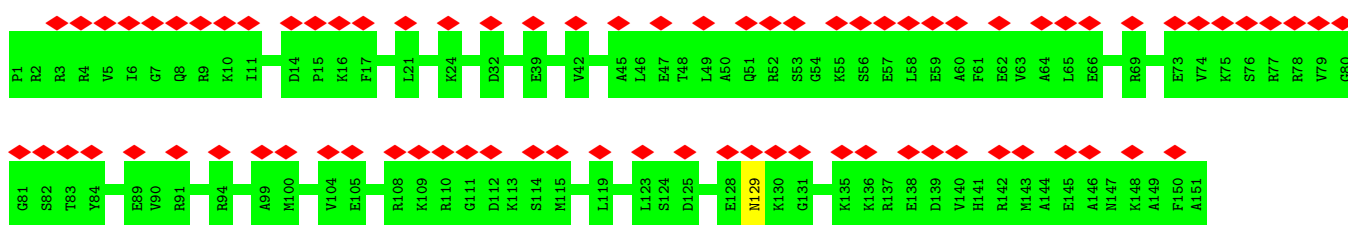
- Molecule 39: 30S ribosomal protein S5



- Molecule 40: 30S ribosomal protein S6

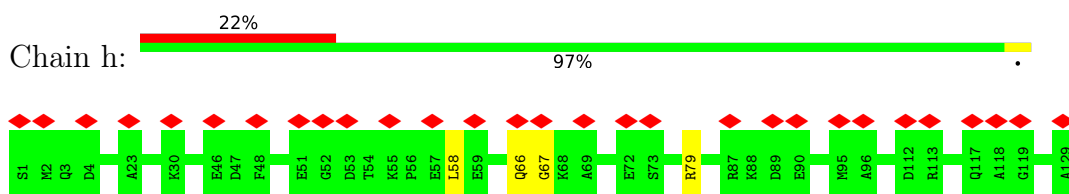


- Molecule 41: 30S ribosomal protein S7

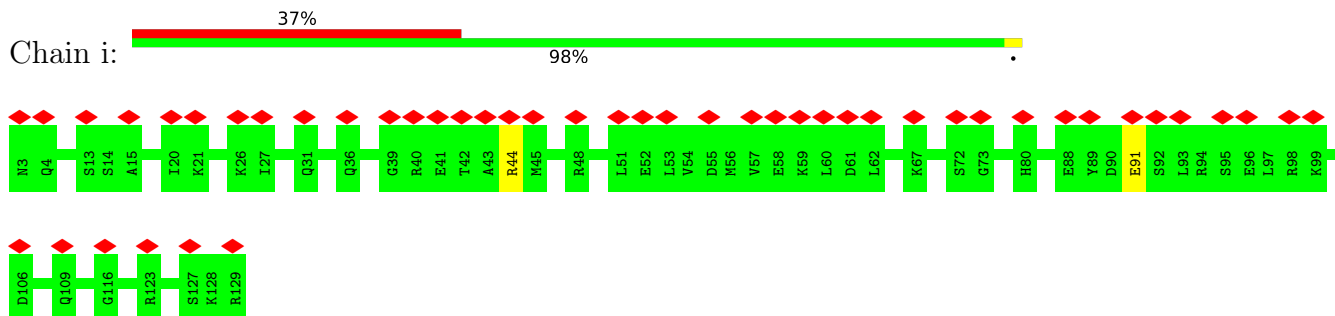


- Molecule 42: 30S ribosomal protein S8

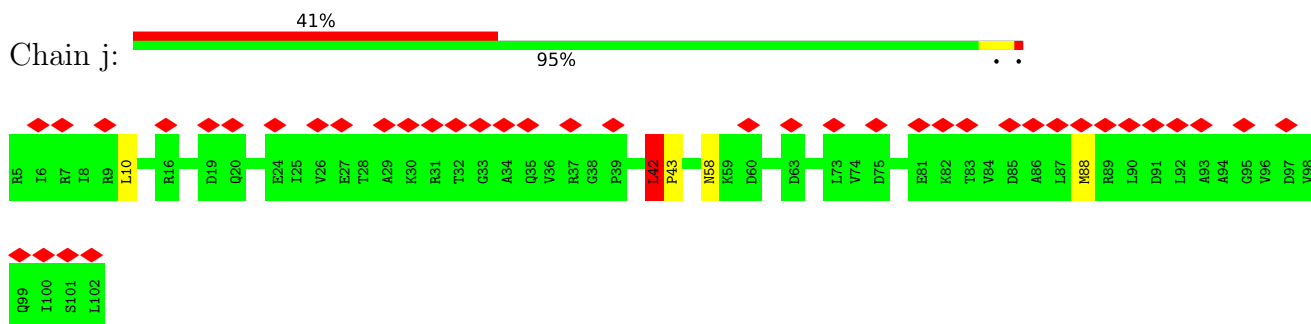




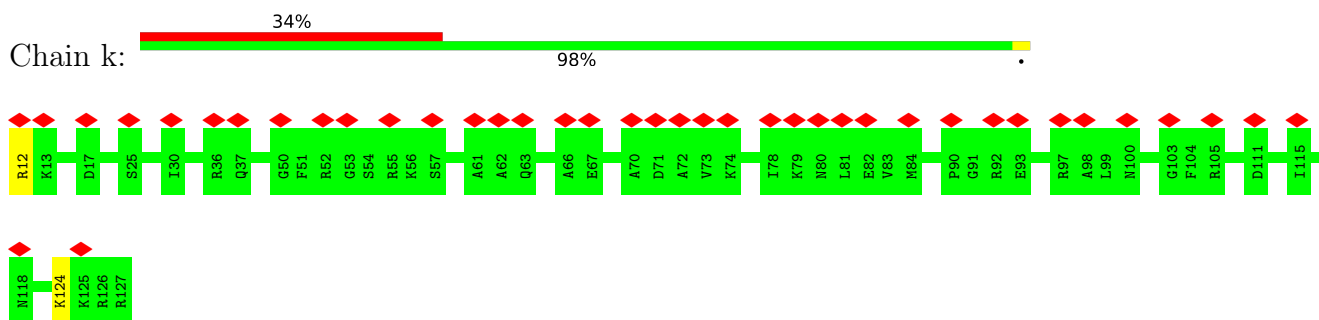
- Molecule 43: 30S ribosomal protein S9



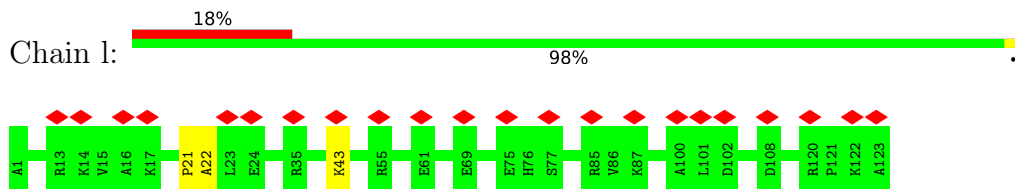
- Molecule 44: 30S ribosomal protein S10



- Molecule 45: 30S ribosomal protein S11

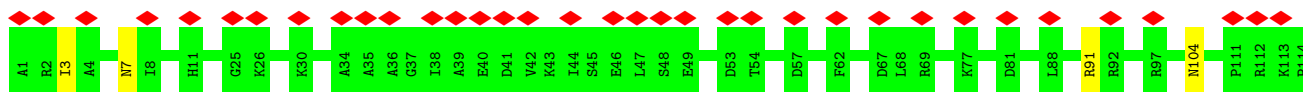


- Molecule 46: 30S ribosomal protein S12

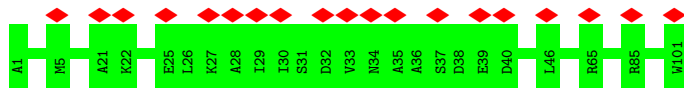


- Molecule 47: 30S ribosomal protein S13

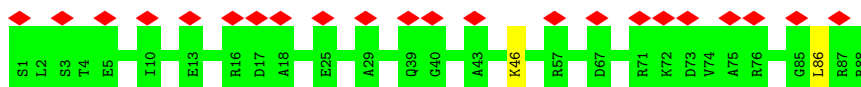




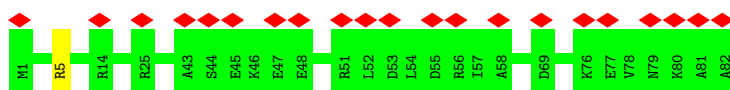
- Molecule 48: 30S ribosomal protein S14



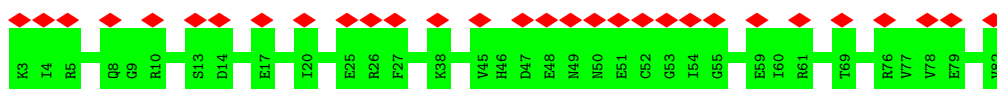
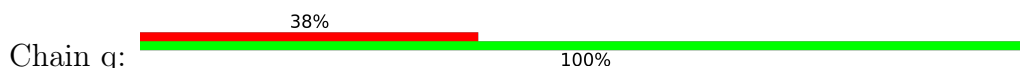
- Molecule 49: 30S ribosomal protein S15



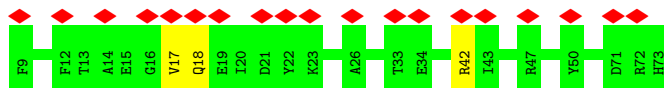
- Molecule 50: 30S ribosomal protein S16



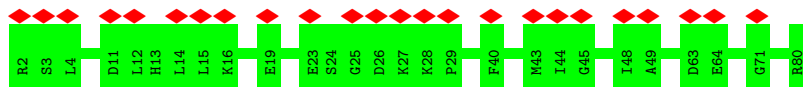
- Molecule 51: 30S ribosomal protein S17



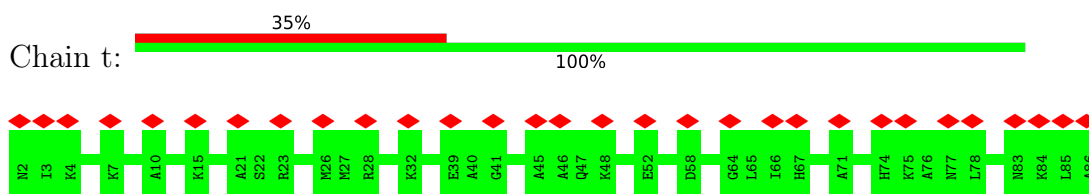
- Molecule 52: 30S ribosomal protein S18



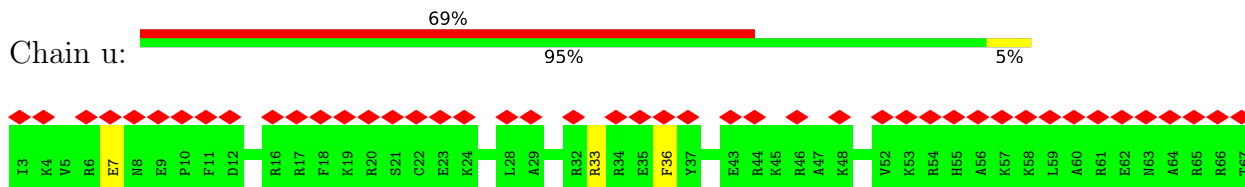
- Molecule 53: 30S ribosomal protein S19



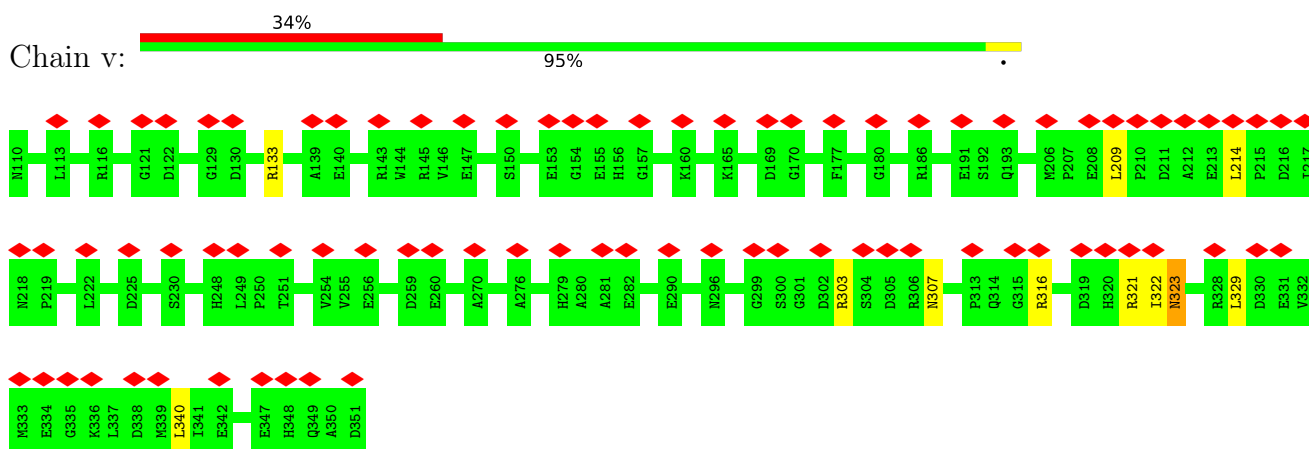
- Molecule 54: 30S ribosomal protein S20



- Molecule 55: 30S ribosomal protein S21



- Molecule 56: Peptide chain release factor RF1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36826	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 ( $e^-/\text{\AA}^2$ )	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	2.131	Depositor
Minimum map value	-1.467	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.407	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	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	A	1.25	33/69734 (0.0%)	1.36	809/108788 (0.7%)
2	B	1.04	1/2876 (0.0%)	1.47	56/4483 (1.2%)
3	C	0.62	0/2121	0.69	0/2852
4	D	0.63	0/1586	0.69	1/2134 (0.0%)
5	E	0.61	1/1571 (0.1%)	0.68	1/2113 (0.0%)
6	F	0.51	0/1434	0.74	3/1926 (0.2%)
7	G	0.47	0/1343	0.65	0/1816
8	H	0.36	0/1122	0.60	1/1515 (0.1%)
9	I	0.35	0/1046	0.67	0/1410
10	J	0.57	0/1152	0.63	0/1551
11	K	0.59	0/947	0.76	0/1268
12	L	0.62	1/1054 (0.1%)	0.79	0/1403
13	M	0.62	0/1093	0.71	1/1460 (0.1%)
14	N	0.58	0/973	0.74	0/1301
15	O	0.56	0/902	0.67	0/1209
16	P	0.60	0/929	0.68	1/1242 (0.1%)
17	Q	0.72	0/960	0.66	0/1278
18	R	0.58	0/829	0.72	0/1107
19	S	0.58	0/864	0.70	0/1156
20	T	0.53	0/744	0.65	0/994
21	U	0.47	0/787	0.66	0/1051
22	V	0.55	0/766	0.65	0/1025
23	W	0.65	0/582	0.63	0/769
24	X	0.53	0/635	0.65	0/848
25	Y	0.41	0/510	0.66	0/677
26	Z	0.53	0/453	0.65	0/605
27	0	0.57	0/450	0.65	0/599
28	1	0.55	0/416	0.66	0/554
29	2	0.62	0/380	0.74	0/498
30	3	0.63	0/513	0.78	1/676 (0.1%)
31	4	0.65	0/303	0.59	0/397
32	5	0.39	0/1001	0.81	1/1350 (0.1%)
33	6	0.40	0/531	0.63	0/709
34	7	1.17	0/166	1.09	0/256

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	a	1.17	5/36967 (0.0%)	1.33	366/57666 (0.6%)
36	b	0.44	0/1735	0.71	0/2338
37	c	0.54	0/1651	0.79	2/2225 (0.1%)
38	d	0.51	0/1665	0.75	3/2227 (0.1%)
39	e	0.59	0/1154	0.76	1/1554 (0.1%)
40	f	0.48	0/835	0.81	2/1128 (0.2%)
41	g	0.46	0/1195	0.68	0/1602
42	h	0.54	0/989	0.78	2/1326 (0.2%)
43	i	0.53	0/1034	0.70	0/1375
44	j	0.50	0/796	0.93	3/1077 (0.3%)
45	k	0.51	0/885	0.69	0/1195
46	l	0.63	0/969	0.77	2/1300 (0.2%)
47	m	0.49	0/892	0.74	0/1193
48	n	0.52	0/811	0.63	0/1081
49	o	0.48	0/722	0.68	1/964 (0.1%)
50	p	0.54	0/659	0.71	0/884
51	q	0.57	0/657	0.73	0/881
52	r	0.53	0/511	0.69	0/689
53	s	0.52	0/652	0.69	0/877
54	t	0.48	0/671	0.66	0/888
55	u	0.43	0/500	0.82	0/668
56	v	0.53	0/1910	0.75	2/2573 (0.1%)
57	x	1.03	0/1841	1.38	26/2869 (0.9%)
58	z	0.40	0/127	0.81	0/175
All	All	1.06	41/160601 (0.0%)	1.21	1285/239775 (0.5%)

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
56	v	0	1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	G	OP3-P	-11.16	1.47	1.61
35	a	2	A	OP3-P	-10.97	1.48	1.61
2	B	1	U	OP3-P	-10.32	1.48	1.61
1	A	1142	A	N9-C4	-7.34	1.33	1.37
5	E	85	PHE	CA-CB	-7.07	1.38	1.53

The worst 5 of 1285 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	j	42	LEU	C-N-CD	-15.77	85.92	120.60
37	c	96	VAL	C-N-CD	-15.69	86.08	120.60
35	a	516	U	N3-C2-O2	-13.84	112.52	122.20
1	A	1917	U	N3-C2-O2	-13.13	113.01	122.20
1	A	2072	C	C6-N1-C2	-13.04	115.08	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	v	303	ARG	Sidechain

## 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	
3	C	269/271 (99%)	242 (90%)	27 (10%)	0	100	100
4	D	207/209 (99%)	182 (88%)	25 (12%)	0	100	100
5	E	199/201 (99%)	182 (92%)	16 (8%)	1 (0%)	29	61
6	F	175/177 (99%)	159 (91%)	16 (9%)	0	100	100
7	G	174/176 (99%)	159 (91%)	14 (8%)	1 (1%)	25	57
8	H	147/149 (99%)	127 (86%)	20 (14%)	0	100	100
9	I	139/141 (99%)	114 (82%)	25 (18%)	0	100	100
10	J	140/142 (99%)	129 (92%)	11 (8%)	0	100	100
11	K	120/122 (98%)	103 (86%)	16 (13%)	1 (1%)	19	51

*Continued on next page...*

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	141/143 (99%)	117 (83%)	23 (16%)	1 (1%)	22	55
13	M	134/136 (98%)	124 (92%)	8 (6%)	2 (2%)	10	36
14	N	118/120 (98%)	105 (89%)	13 (11%)	0	100	100
15	O	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
16	P	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
17	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
18	R	101/103 (98%)	87 (86%)	13 (13%)	1 (1%)	15	46
19	S	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	17	49
20	T	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
21	U	100/102 (98%)	84 (84%)	16 (16%)	0	100	100
22	V	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
23	W	73/75 (97%)	66 (90%)	7 (10%)	0	100	100
24	X	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
25	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
26	Z	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
27	0	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
28	1	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
29	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
30	3	62/64 (97%)	54 (87%)	8 (13%)	0	100	100
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	101 (78%)	27 (21%)	1 (1%)	19	51
33	6	64/66 (97%)	53 (83%)	11 (17%)	0	100	100
36	b	216/218 (99%)	177 (82%)	37 (17%)	2 (1%)	17	49
37	c	204/206 (99%)	183 (90%)	18 (9%)	3 (2%)	10	36
38	d	203/205 (99%)	180 (89%)	23 (11%)	0	100	100
39	e	155/157 (99%)	136 (88%)	19 (12%)	0	100	100
40	f	98/100 (98%)	82 (84%)	15 (15%)	1 (1%)	15	46
41	g	149/151 (99%)	134 (90%)	14 (9%)	1 (1%)	22	55
42	h	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	19	51
43	i	125/127 (98%)	105 (84%)	19 (15%)	1 (1%)	19	51
44	j	96/98 (98%)	79 (82%)	15 (16%)	2 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	k	114/116 (98%)	91 (80%)	23 (20%)	0	100	100
46	l	121/123 (98%)	94 (78%)	26 (22%)	1 (1%)	19	51
47	m	112/114 (98%)	98 (88%)	13 (12%)	1 (1%)	17	49
48	n	99/101 (98%)	88 (89%)	11 (11%)	0	100	100
49	o	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	13	41
50	p	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
51	q	78/80 (98%)	62 (80%)	16 (20%)	0	100	100
52	r	63/65 (97%)	50 (79%)	11 (18%)	2 (3%)	4	22
53	s	77/79 (98%)	69 (90%)	8 (10%)	0	100	100
54	t	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
55	u	63/65 (97%)	43 (68%)	17 (27%)	3 (5%)	2	15
56	v	240/242 (99%)	213 (89%)	24 (10%)	3 (1%)	12	39
58	z	12/14 (86%)	10 (83%)	1 (8%)	1 (8%)	1	5
All	All	6099/6205 (98%)	5361 (88%)	706 (12%)	32 (0%)	32	61

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	175	LYS
18	R	54	VAL
32	5	80	THR
36	b	19	THR
37	c	96	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	
3	C	216/216 (100%)	214 (99%)	2 (1%)	78	90
4	D	164/164 (100%)	162 (99%)	2 (1%)	71	85
5	E	165/165 (100%)	163 (99%)	2 (1%)	71	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	148/148 (100%)	148 (100%)	0	100	100
7	G	137/137 (100%)	135 (98%)	2 (2%)	65	82
8	H	114/114 (100%)	114 (100%)	0	100	100
9	I	109/109 (100%)	107 (98%)	2 (2%)	59	79
10	J	116/116 (100%)	116 (100%)	0	100	100
11	K	103/103 (100%)	103 (100%)	0	100	100
12	L	102/102 (100%)	101 (99%)	1 (1%)	76	88
13	M	109/109 (100%)	108 (99%)	1 (1%)	78	90
14	N	100/100 (100%)	99 (99%)	1 (1%)	76	88
15	O	86/86 (100%)	86 (100%)	0	100	100
16	P	99/99 (100%)	98 (99%)	1 (1%)	76	88
17	Q	89/89 (100%)	88 (99%)	1 (1%)	73	86
18	R	84/84 (100%)	83 (99%)	1 (1%)	71	85
19	S	93/93 (100%)	93 (100%)	0	100	100
20	T	80/80 (100%)	80 (100%)	0	100	100
21	U	83/83 (100%)	83 (100%)	0	100	100
22	V	78/78 (100%)	78 (100%)	0	100	100
23	W	57/57 (100%)	56 (98%)	1 (2%)	59	79
24	X	67/67 (100%)	66 (98%)	1 (2%)	65	82
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	48/48 (100%)	48 (100%)	0	100	100
27	0	47/47 (100%)	47 (100%)	0	100	100
28	1	45/45 (100%)	45 (100%)	0	100	100
29	2	38/38 (100%)	38 (100%)	0	100	100
30	3	51/51 (100%)	51 (100%)	0	100	100
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	100 (100%)	0	100	100
33	6	59/59 (100%)	59 (100%)	0	100	100
36	b	180/180 (100%)	176 (98%)	4 (2%)	52	75
37	c	170/170 (100%)	167 (98%)	3 (2%)	59	79
38	d	172/172 (100%)	167 (97%)	5 (3%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	e	114/119 (96%)	112 (98%)	2 (2%)	59	79
40	f	87/87 (100%)	86 (99%)	1 (1%)	73	86
41	g	124/124 (100%)	124 (100%)	0	100	100
42	h	104/104 (100%)	103 (99%)	1 (1%)	76	88
43	i	105/105 (100%)	104 (99%)	1 (1%)	76	88
44	j	86/86 (100%)	84 (98%)	2 (2%)	50	74
45	k	89/89 (100%)	87 (98%)	2 (2%)	52	75
46	l	103/103 (100%)	103 (100%)	0	100	100
47	m	92/92 (100%)	89 (97%)	3 (3%)	38	66
48	n	79/83 (95%)	79 (100%)	0	100	100
49	o	76/76 (100%)	76 (100%)	0	100	100
50	p	65/65 (100%)	64 (98%)	1 (2%)	65	82
51	q	74/74 (100%)	74 (100%)	0	100	100
52	r	48/56 (86%)	47 (98%)	1 (2%)	53	76
53	s	70/70 (100%)	70 (100%)	0	100	100
54	t	65/65 (100%)	65 (100%)	0	100	100
55	u	44/55 (80%)	44 (100%)	0	100	100
56	v	195/195 (100%)	189 (97%)	6 (3%)	40	68
58	z	14/14 (100%)	13 (93%)	1 (7%)	14	44
All	All	5032/5060 (99%)	4981 (99%)	51 (1%)	77	88

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	d	183	ARG
44	j	42	LEU
56	v	340	LEU
38	d	190	LEU
40	f	53	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
30	3	42	HIS

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Mol	Chain	Res	Type
47	m	99	GLN
36	b	121	GLN
47	m	7	ASN
52	r	51	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2898/2903 (99%)	681 (23%)	27 (0%)
2	B	119/120 (99%)	30 (25%)	5 (4%)
34	7	6/7 (85%)	4 (66%)	0
35	a	1538/1539 (99%)	345 (22%)	0
57	x	76/77 (98%)	21 (27%)	0
All	All	4637/4646 (99%)	1081 (23%)	32 (0%)

5 of 1081 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	10	A
1	A	12	U
1	A	14	A
1	A	23	G

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	12	C
2	B	52	A
1	A	1022	G
1	A	1020	A
2	B	66	A

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	60:ARG	C	61:LEU	N	1.18

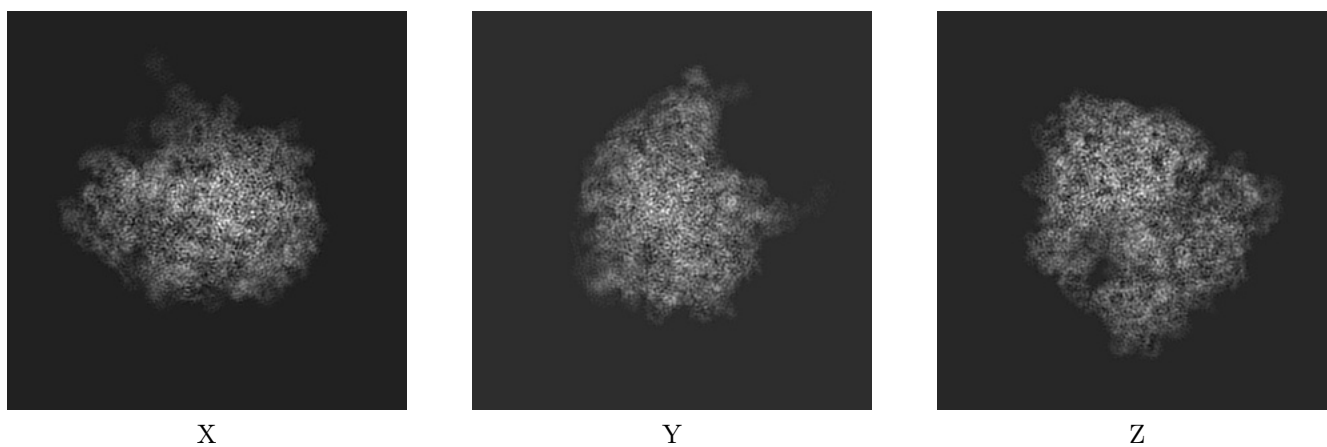
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3730. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections [i](#)

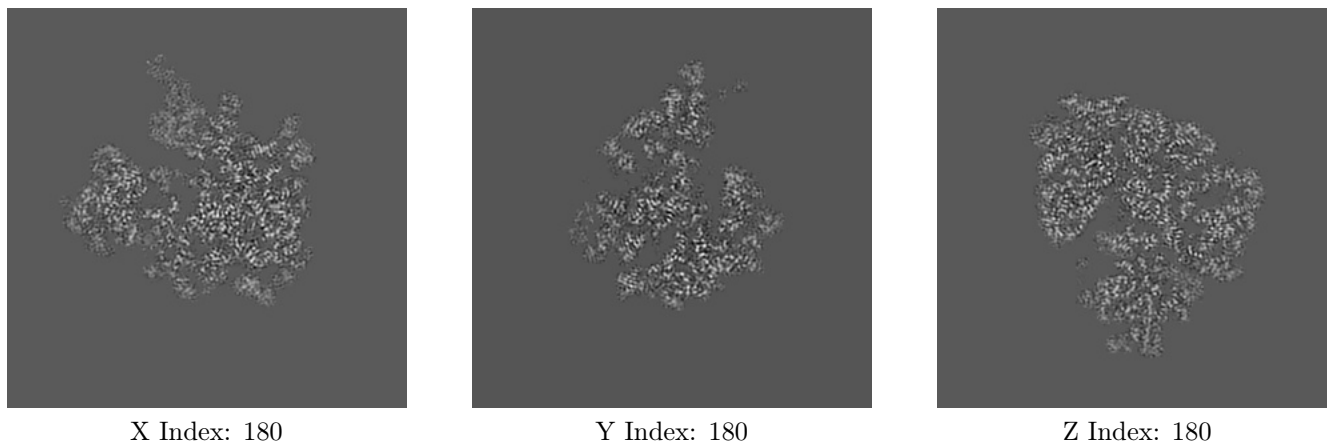
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

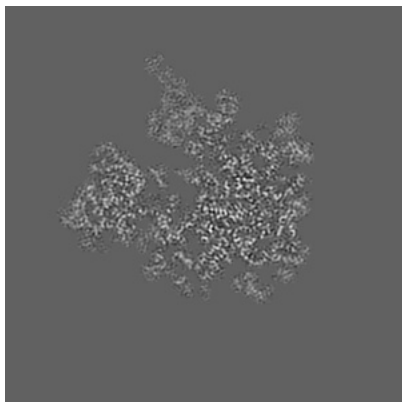
#### 6.2.1 Primary map



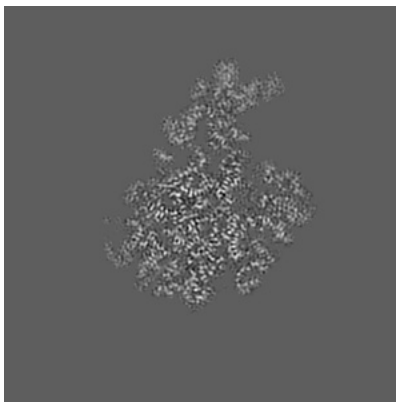
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

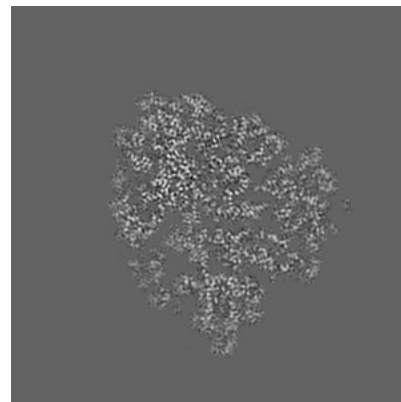
### 6.3.1 Primary map



X Index: 178



Y Index: 190

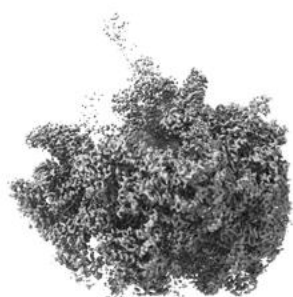


Z Index: 186

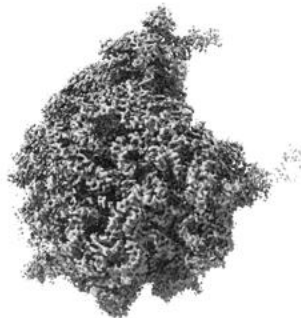
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

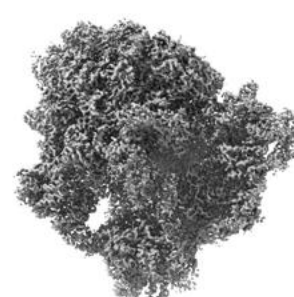
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.407. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

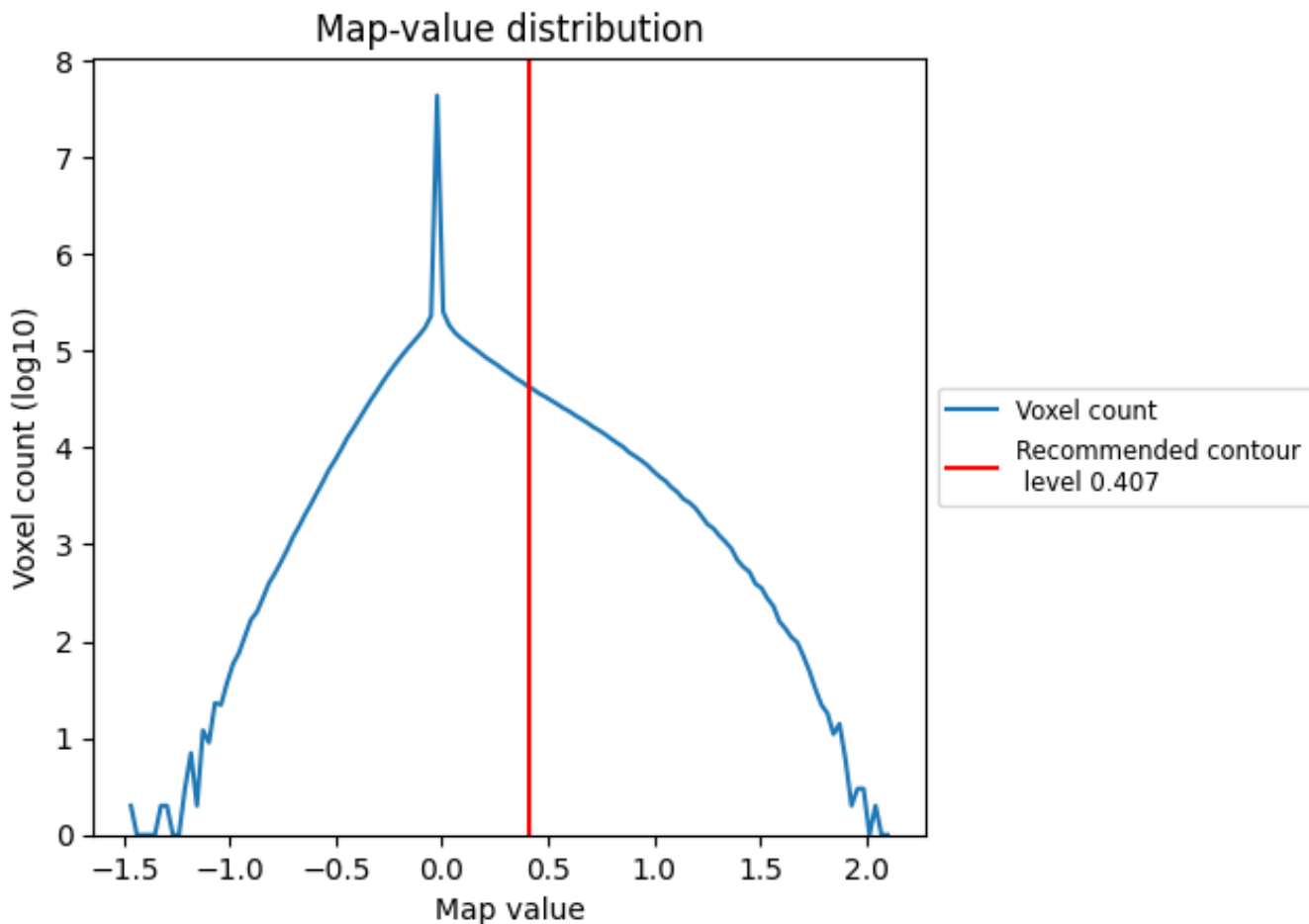
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

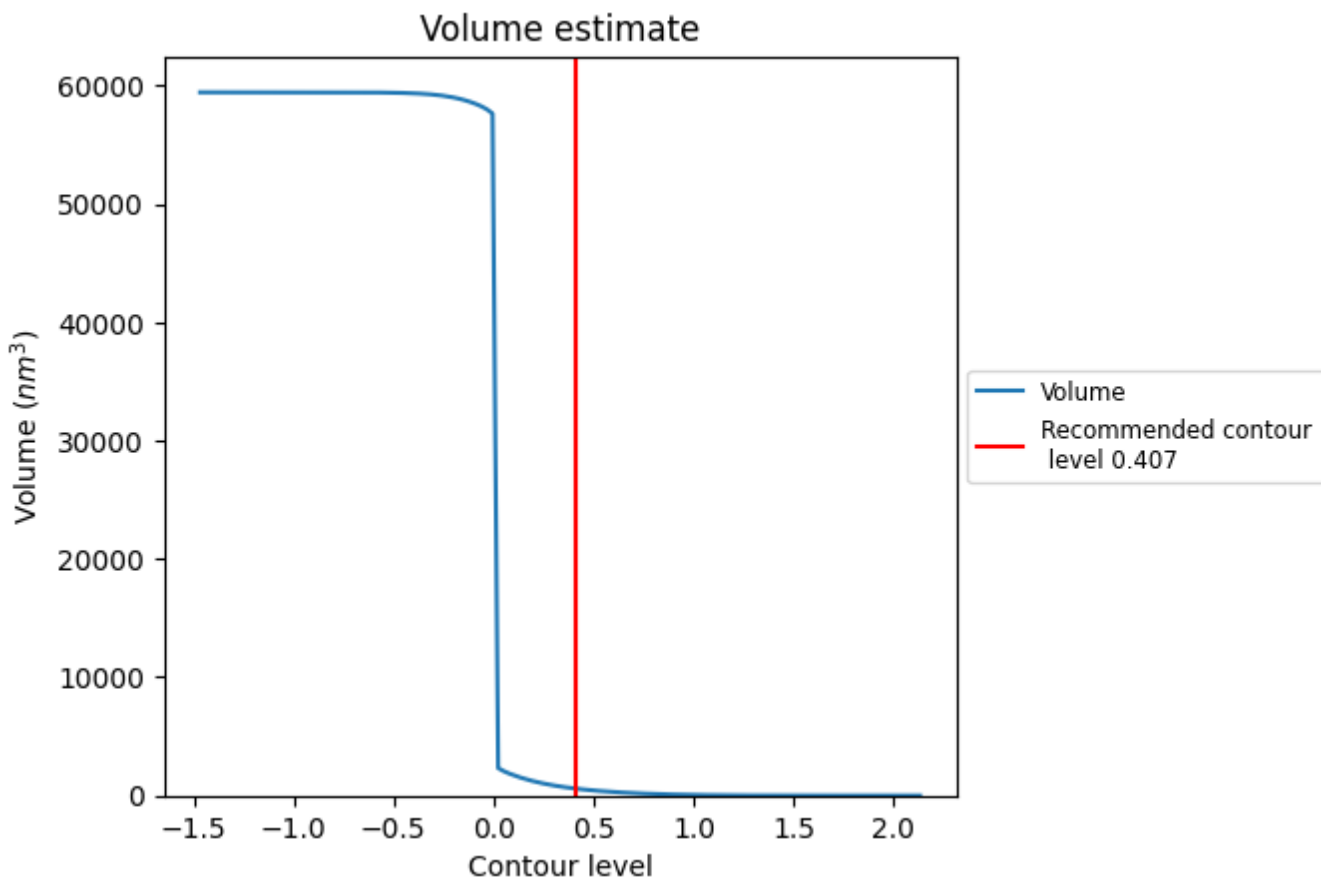
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

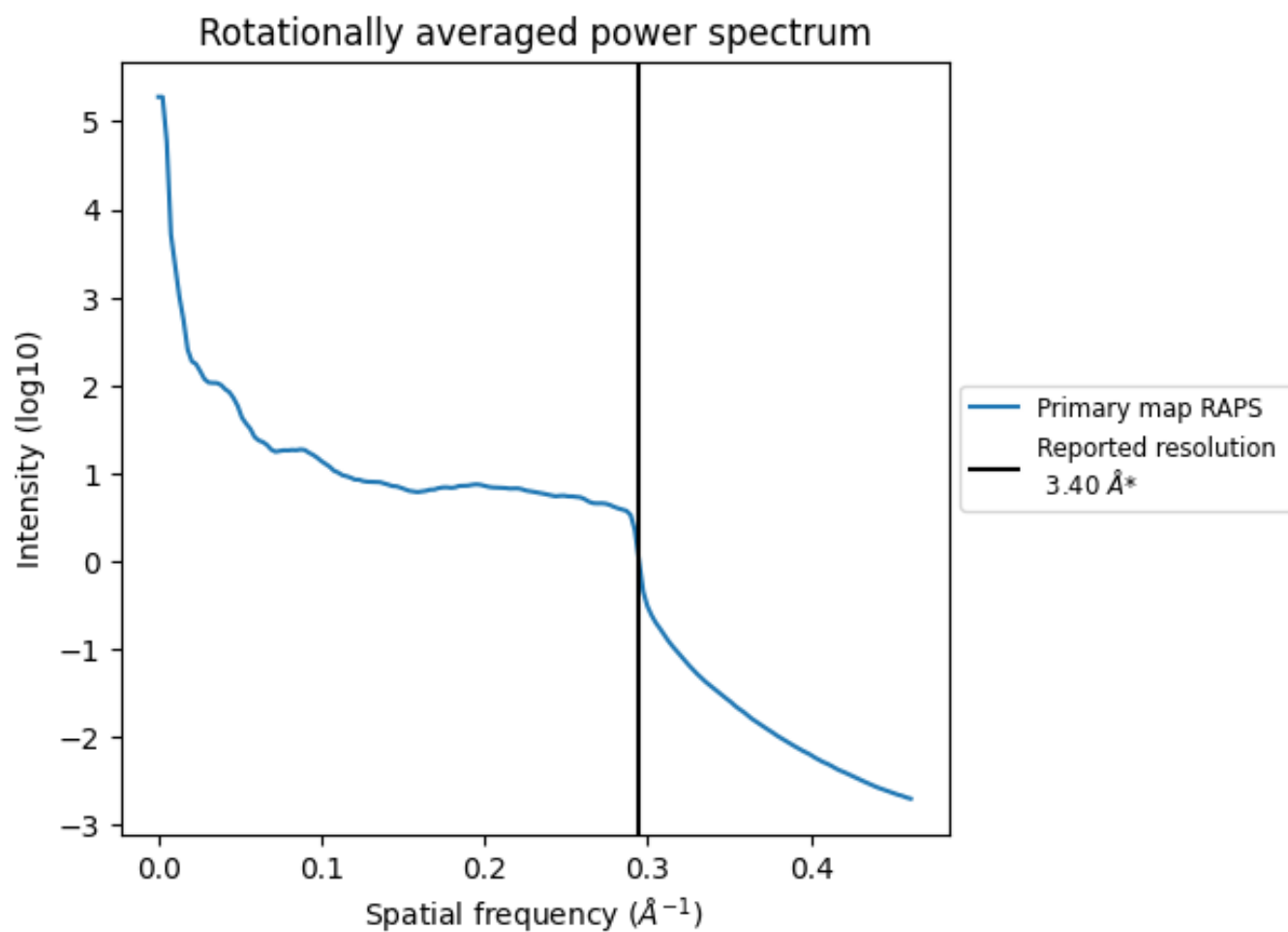
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 595 nm<sup>3</sup>; this corresponds to an approximate mass of 537 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.294 \text{\AA}^{-1}$

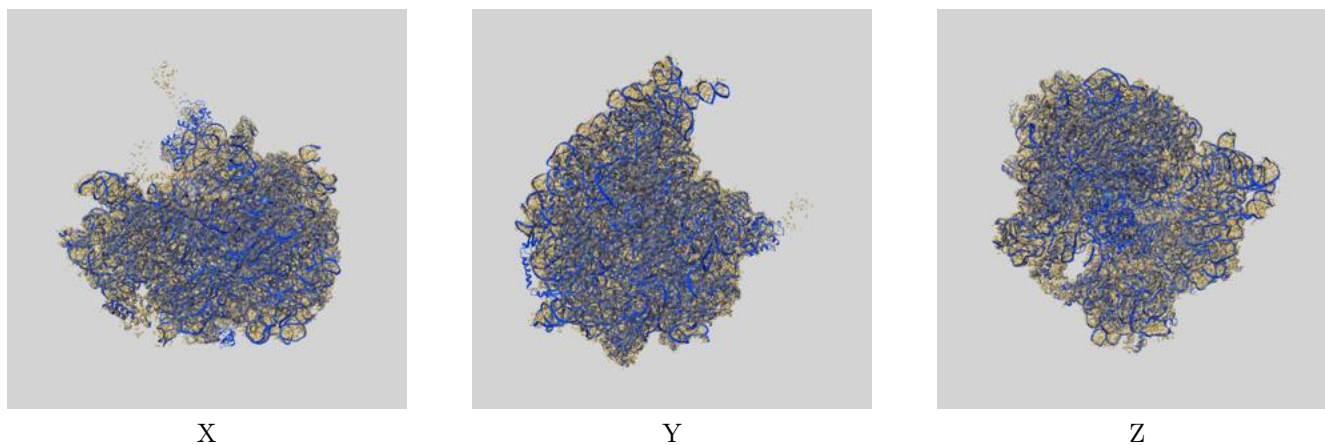
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

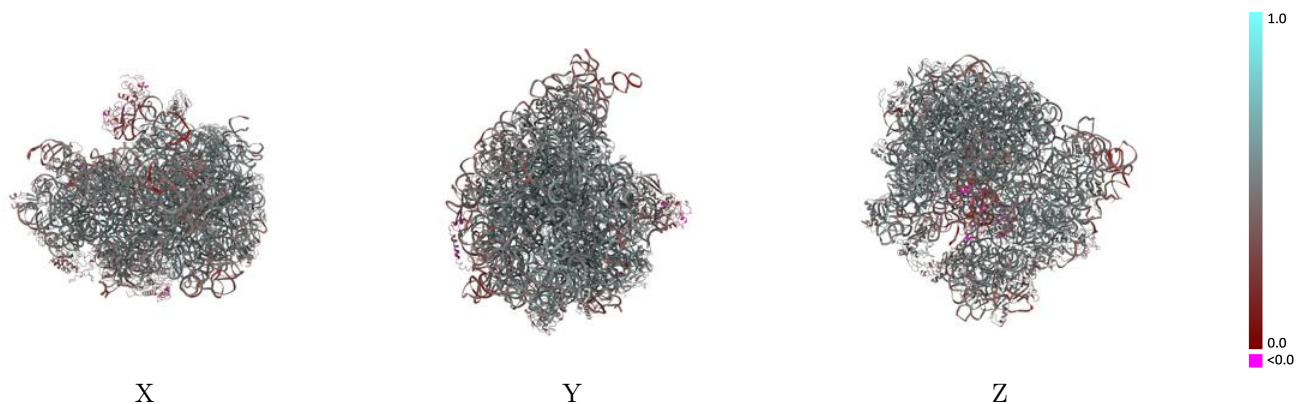
This section contains information regarding the fit between EMDB map EMD-3730 and PDB model 5O2R. Per-residue inclusion information can be found in section 3 on page 14.

### 9.1 Map-model overlay [i](#)



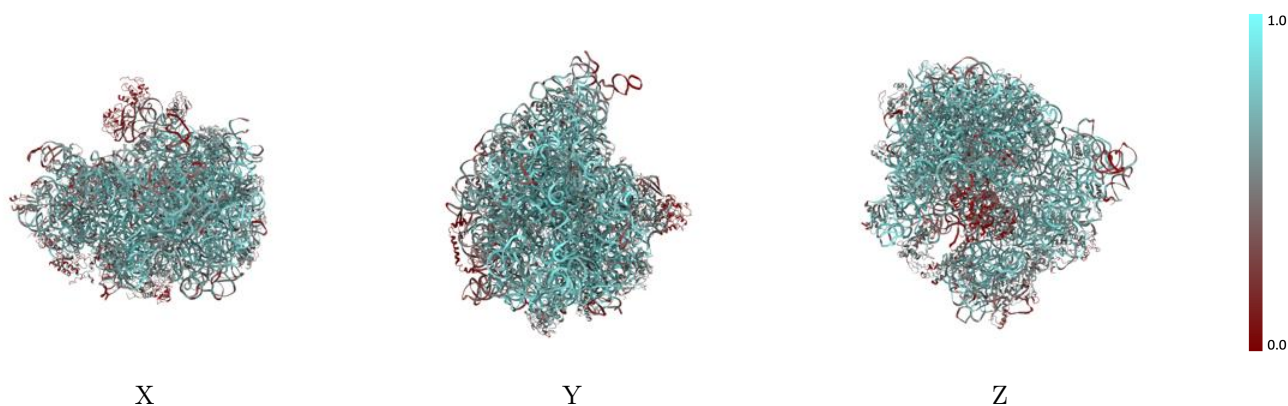
The images above show the 3D surface view of the map at the recommended contour level 0.407 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



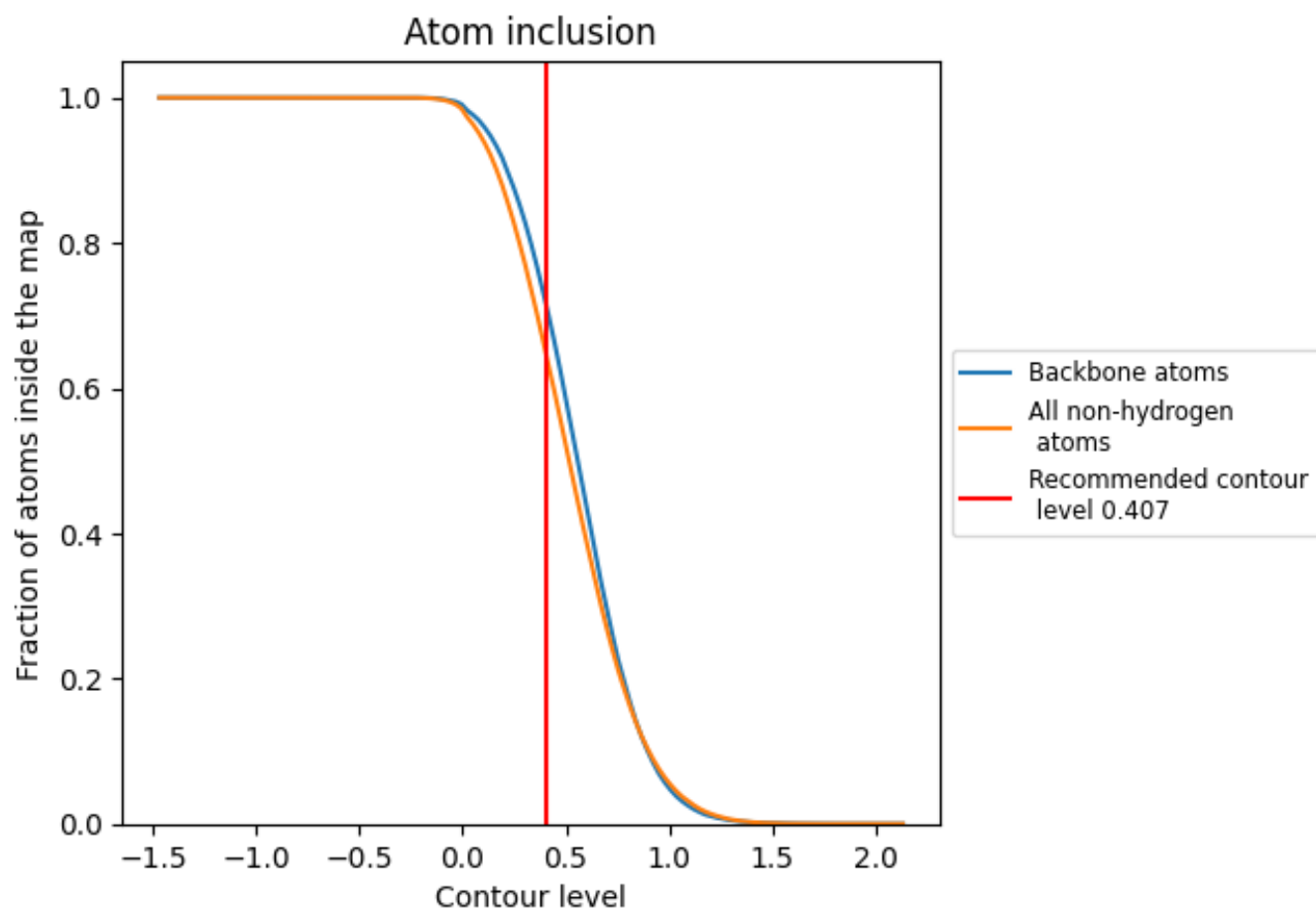
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.407).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.407) and Q-score for the entire model and for each chain.

















































Chain	Atom inclusion	Q-score
All	 0.6430	 0.4760
0	 0.6098	 0.5100
1	 0.5012	 0.4880
2	 0.6789	 0.5170
3	 0.6721	 0.5400
4	 0.5753	 0.5170
5	 0.0682	 0.2130
6	 0.3523	 0.3920
7	 0.8121	 0.5450
A	 0.7198	 0.4880
B	 0.7076	 0.4730
C	 0.6042	 0.5210
D	 0.5982	 0.5120
E	 0.5526	 0.4840
F	 0.4836	 0.4530
G	 0.3763	 0.4170
H	 0.1122	 0.2790
I	 0.0616	 0.2140
J	 0.5973	 0.5110
K	 0.5816	 0.5030
L	 0.5837	 0.5060
M	 0.5969	 0.5180
N	 0.6410	 0.5220
O	 0.5423	 0.4760
P	 0.5833	 0.5040
Q	 0.6564	 0.5180
R	 0.5521	 0.4840
S	 0.6005	 0.5050
T	 0.5277	 0.4810
U	 0.4889	 0.4640
V	 0.5461	 0.4820
W	 0.6440	 0.5380
X	 0.5474	 0.4820
Y	 0.4447	 0.4330
Z	 0.6133	 0.5050



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Chain	Atom inclusion	Q-score
a	 0.7026	 0.4770
b	 0.3552	 0.3970
c	 0.5209	 0.4600
d	 0.4428	 0.4240
e	 0.5862	 0.4980
f	 0.4334	 0.4270
g	 0.3934	 0.4250
h	 0.5385	 0.4820
i	 0.4709	 0.4450
j	 0.4389	 0.4410
k	 0.4959	 0.4620
l	 0.5787	 0.4960
m	 0.4853	 0.4370
n	 0.5664	 0.4680
o	 0.5435	 0.4700
p	 0.5295	 0.4710
q	 0.4699	 0.4610
r	 0.5381	 0.4760
s	 0.5040	 0.4620
t	 0.5031	 0.4530
u	 0.3130	 0.3610
v	 0.5063	 0.4820
x	 0.6132	 0.4550
z	 0.4779	 0.4720