



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 02:44 pm GMT

PDB ID : 5ND8
EMDB ID : EMD-3624
Title : Hibernating ribosome from Staphylococcus aureus (Unrotated state)
Authors : Khusainov, I.; Vicens, Q.; Ayupov, R.; Usachev, K.; Myasnikov, A.; Simonetti, A.; Validov, S.; Kieffer, B.; Yusupova, G.; Yusupov, M.; Hashem, Y.
Deposited on : 2017-03-07
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

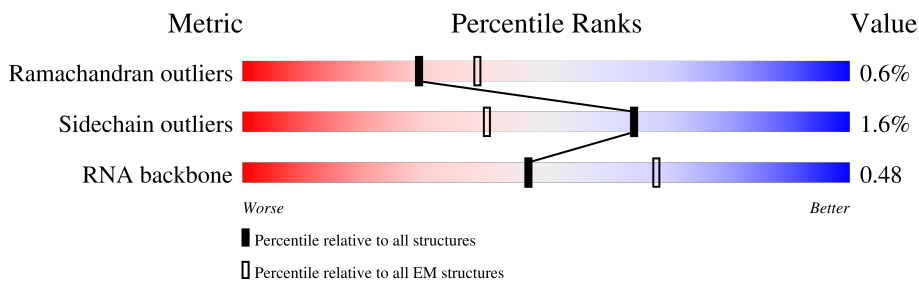
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	a	1547	
2	b	255	
3	c	217	
4	d	200	
5	e	166	
6	f	98	
7	g	156	
8	h	132	

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Mol	Chain	Length	Quality of chain
9	i	132	57% 97%
10	j	102	68% 96%
11	k	129	40% 91% 9%
12	l	137	23% 96%
13	m	121	55% 88% 9%
14	n	61	61% 95%
15	o	89	18% 98%
16	p	91	19% 97%
17	q	87	24% 97%
18	r	80	24% 70% 28%
19	s	92	43% 88% 11%
20	t	83	10% 95%
21	u	58	72% 81% 19%
22	v	190	41% 41% 7% 48%
23	A	2918	5% 73% 25%
24	B	114	80% 20%
25	D	277	11% 99%
26	E	220	7% 96%
27	F	207	5% 96%
28	G	179	32% 91% 7%
29	H	178	19% 92% 8%
30	M	145	9% 99%
31	N	122	11% 97%
32	O	146	8% 86% 10%
33	P	144	10% 79% 12% 8%

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Mol	Chain	Length	Quality of chain
34	Q	122	8% 95%
35	R	119	16% 99%
36	S	116	10% 88% 8%
37	T	118	97%
38	U	102	11% 97%
39	V	117	5% 95%
40	W	91	10% 95%
41	X	105	5% 81% 17%
42	Y	217	35% 43% 57%
43	Z	94	5% 69% 11% 19%
44	0	62	19% 71% 26%
45	1	69	7% 93% 6%
46	2	59	7% 97%
47	3	84	60% 95%
48	4	58	16% 74% 26%
49	5	49	43% 53% 43%
50	6	45	91%
51	7	66	8% 85% 6% 9%
52	8	37	14% 97%

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 141043 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1542	33026	14745	6024	10715	1542	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	222	1789	1139	313	330	7	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	204	1609	1012	302	293	2	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	197	1600	1009	300	289	2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	159	1185	745	217	221	2	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	94	781	494	137	147	3	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	143	1142	712	216	210	4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	131	1032	652	183	193	4	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	128	1017	629	203	184	1	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	99	791	498	144	147	2	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	118	880	543	169	165	3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	135	1058	658	214	184	2	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	110	877	537	175	164	1	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			502	317	100	80	5		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			738	454	153	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	85	Total	C	N	O	S	0	0
			698	441	125	131	1		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	58	Total	C	N	O	S	0	0
			478	303	90	83	2		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	82	Total	C	N	O	S	0	0
			661	426	118	115	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	u	47	396	243	82	71	0	0

- Molecule 22 is a protein called Ribosome hibernation promotion factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	v	98	808	506	150	152	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	A	2912	62440	27876	11422	20230	2912	0	0

- Molecule 24 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	B	114	2430	1086	436	794	114	0	0

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	D	275	2103	1309	417	372	5	0	0

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	E	218	1649	1030	304	310	5	0	0

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	F	199	1524	955	281	286	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	G	166	1311	832	223	250	6	0	0

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	H	164	1284	799	232	250	3	0	0

- Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	M	145	1151	717	211	220	3	0	0

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	N	122	920	572	174	170	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	O	131	997	618	197	181	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	P	132	1056	676	202	175	3	0	0

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Q	117	924	564	179	180	1	0	0

- Molecule 35 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	R	119	922	574	174	173	1	0	0

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	S	107	862	544	173	145		0	0

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	T	116	943	593	189	157	4	0	0

- Molecule 38 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	U	102	799	506	142	150	1	0	0

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	V	112	862	537	164	158	3	0	0

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	W	89	725	457	130	134	4	0	0

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	X	87	668	423	122	122	1	0	0

- Molecule 42 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	Z	76	Total	C	N	O	0	0
			585	361	114	110		

- Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	0	46	Total	C	N	O	0	0
			373	231	83	59		

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	1	65	Total	C	N	O	0	0
			536	330	101	105		

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	2	57	Total	C	N	O	0	0
			441	274	83	84		

- Molecule 47 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	83	Total	C	N	O	S	0	0
			677	430	116	128	3		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	43	Total	C	N	O	S	0	0
			351	214	76	57	4		

- Molecule 49 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5	28	Total	C	N	O	S	0	0
			229	137	45	43	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	6	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	7	60	Total	C	N	O	S	0	0
			487	300	108	77	2		

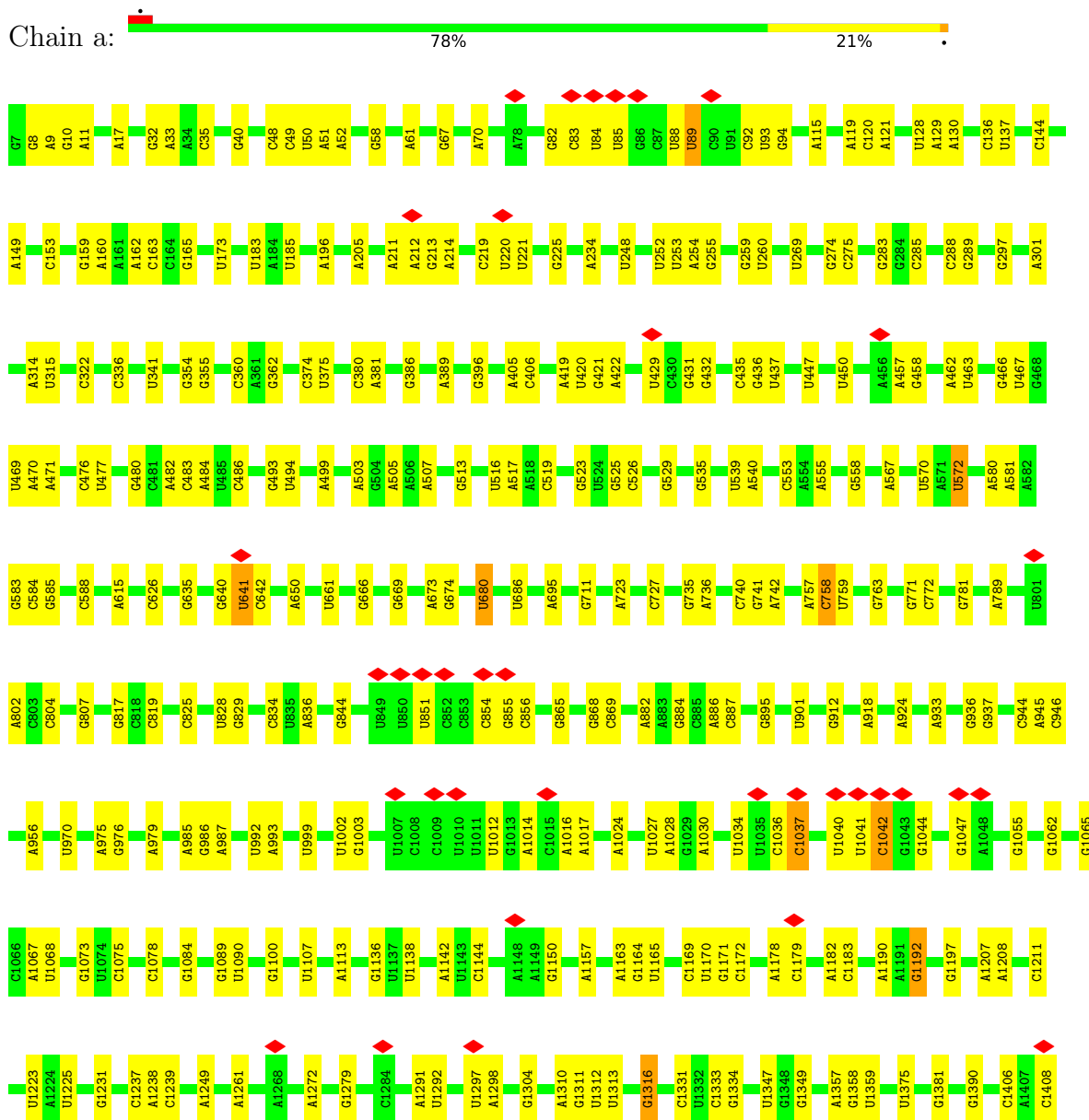
- Molecule 52 is a protein called 50S ribosomal protein L36.

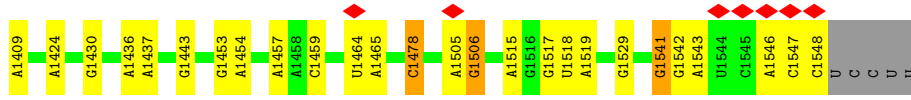
Mol	Chain	Residues	Atoms					AltConf	Trace
52	8	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

3 Residue-property plots [i](#)

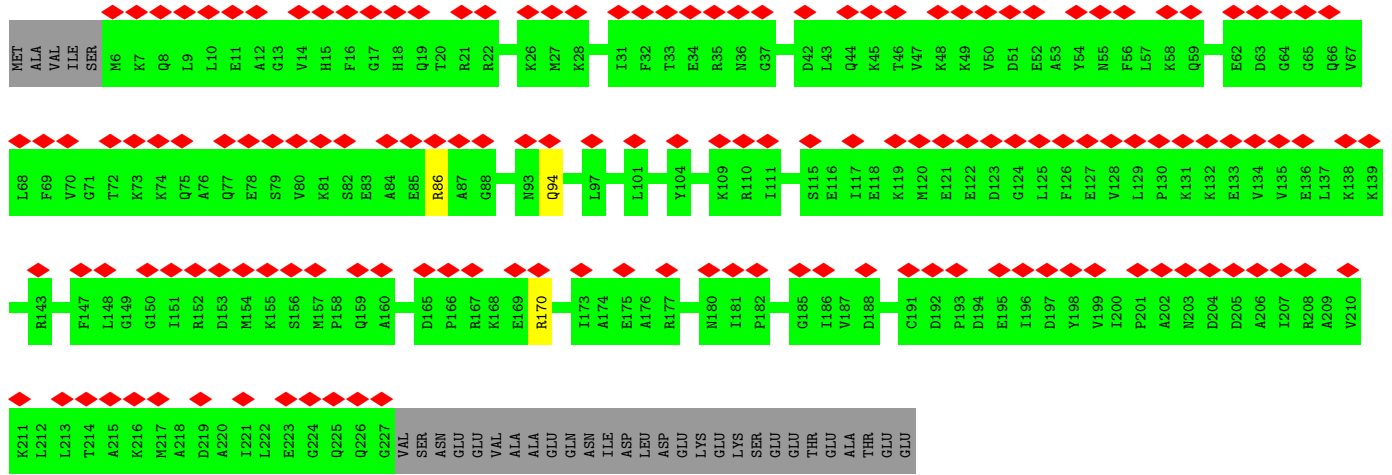
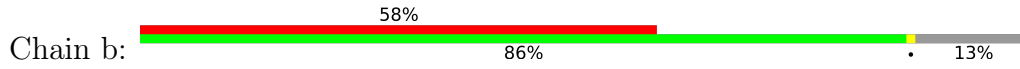
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 ribosomal RNA

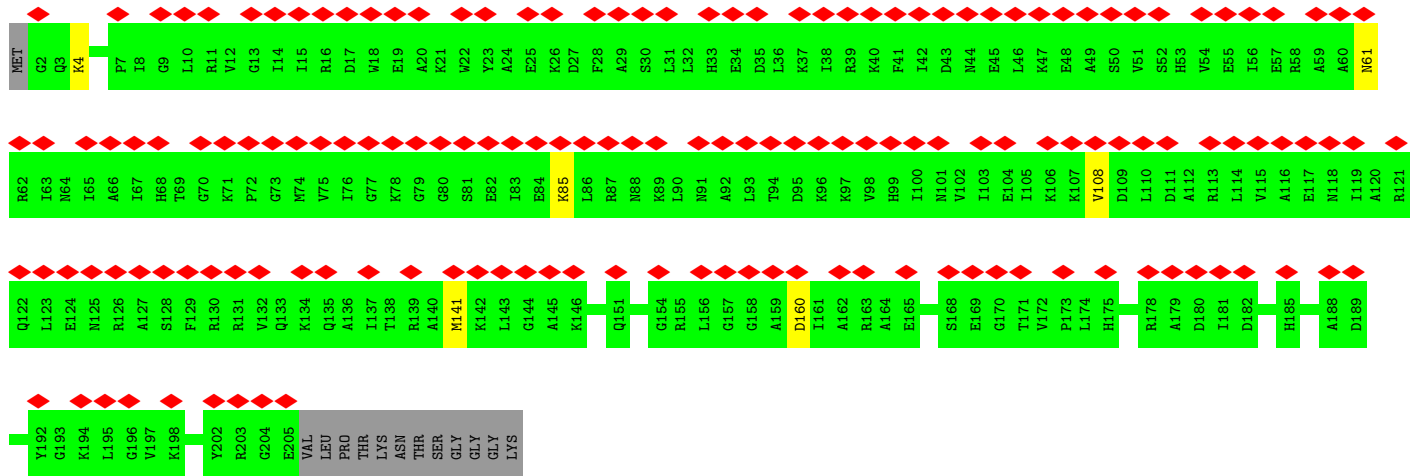
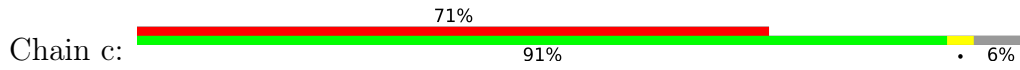




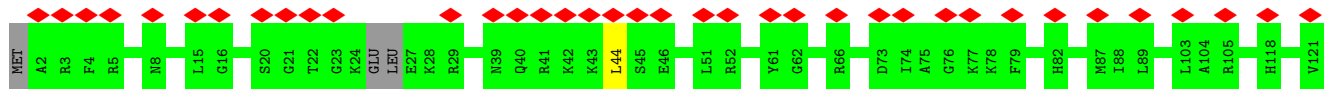
• Molecule 2: 30S ribosomal protein S2

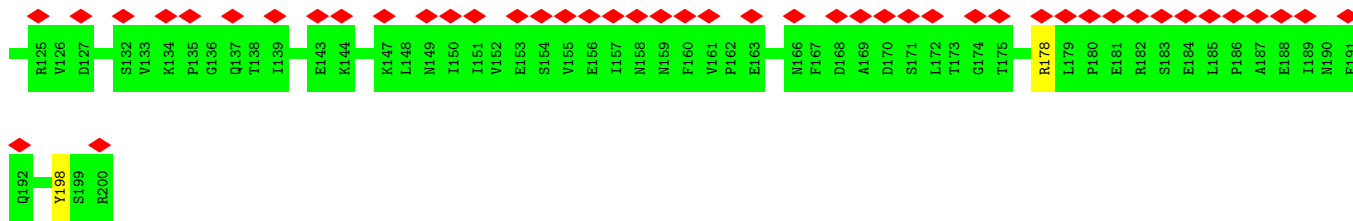


• Molecule 3: 30S ribosomal protein S3

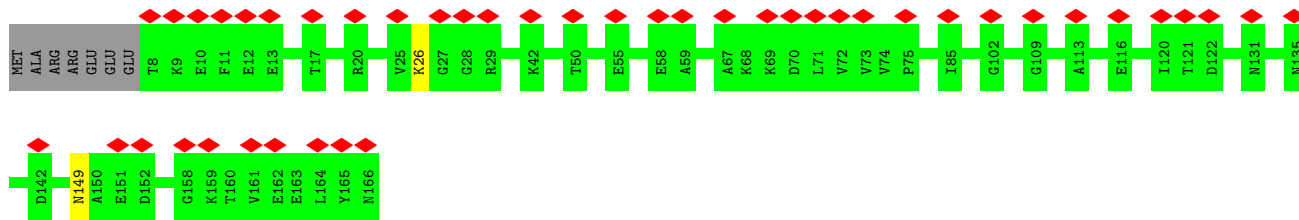


• Molecule 4: 30S ribosomal protein S4

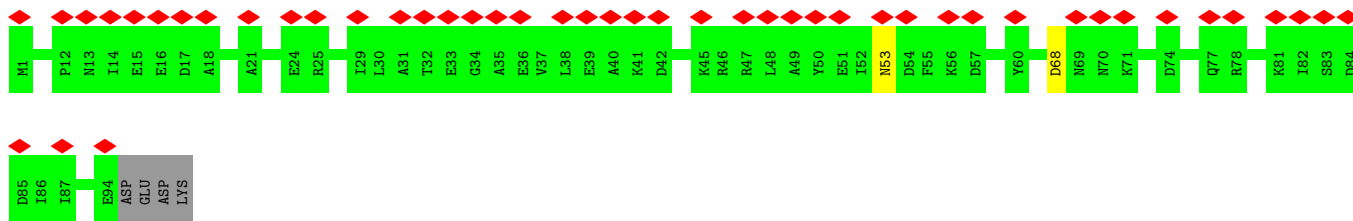
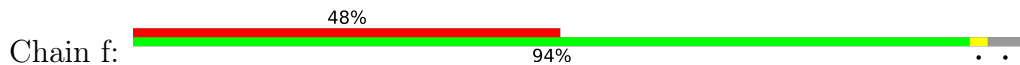




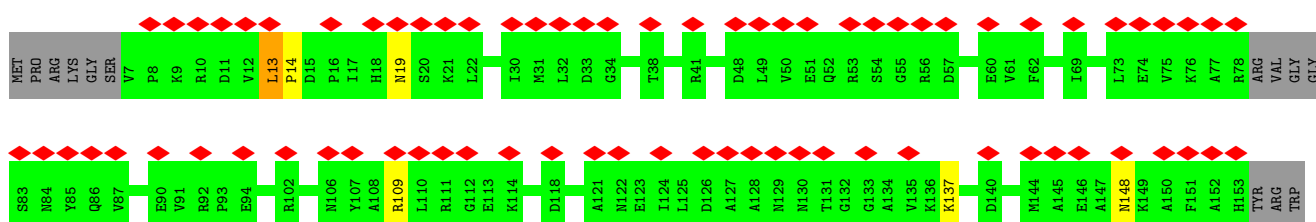
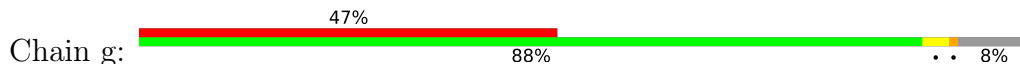
• Molecule 5: 30S ribosomal protein S5



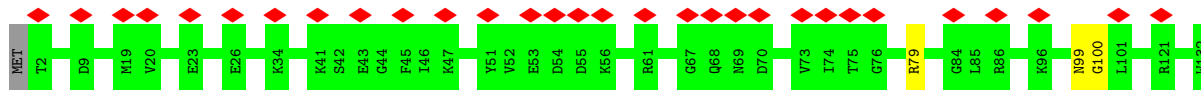
• Molecule 6: 30S ribosomal protein S6



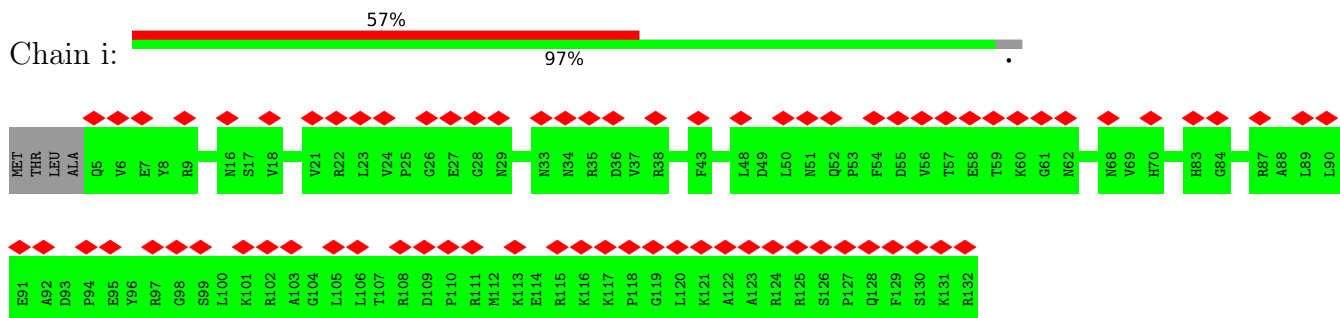
• Molecule 7: 30S ribosomal protein S7



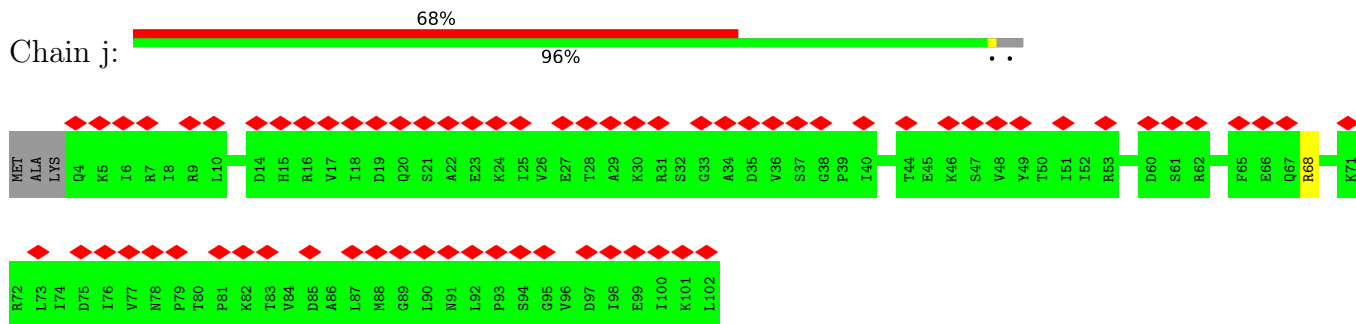
• Molecule 8: 30S ribosomal protein S8



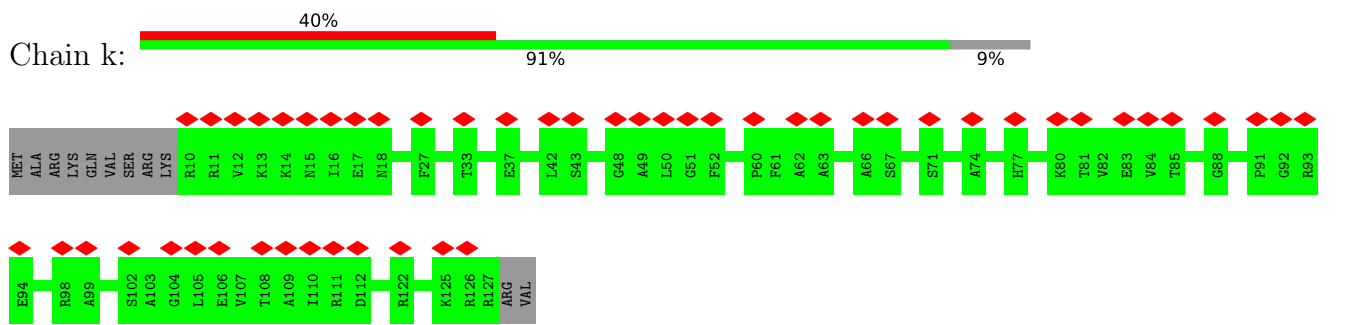
• Molecule 9: 30S ribosomal protein S9



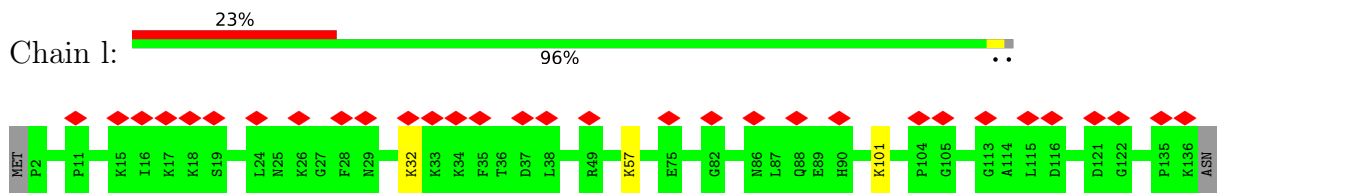
• Molecule 10: 30S ribosomal protein S10



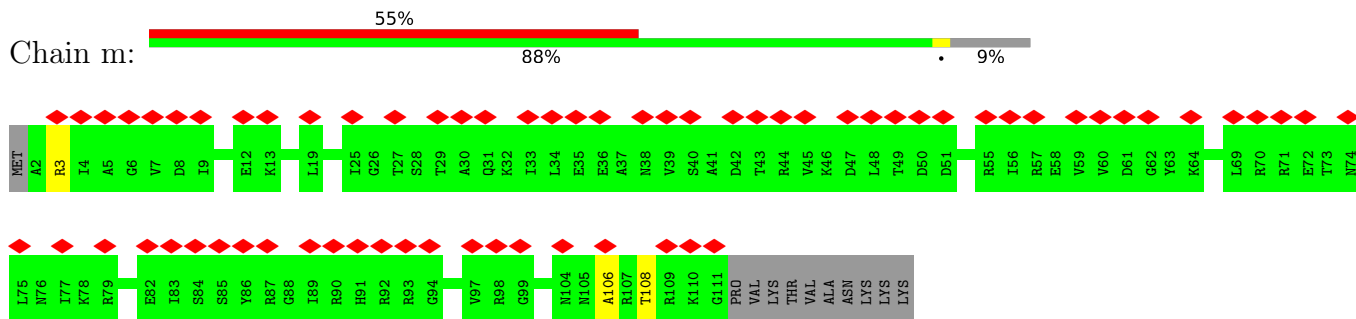
• Molecule 11: 30S ribosomal protein S11



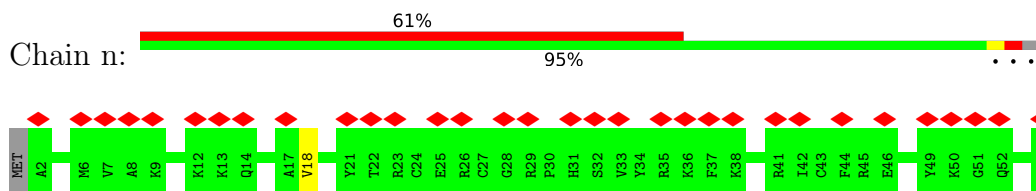
• Molecule 12: 30S ribosomal protein S12



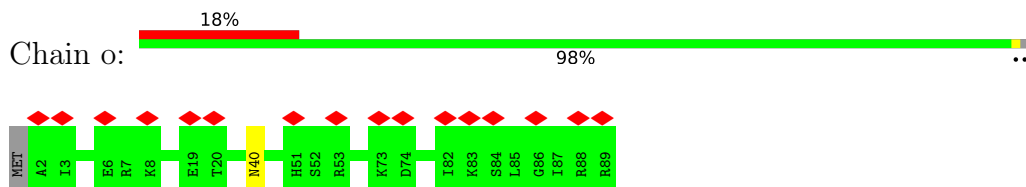
• Molecule 13: 30S ribosomal protein S13



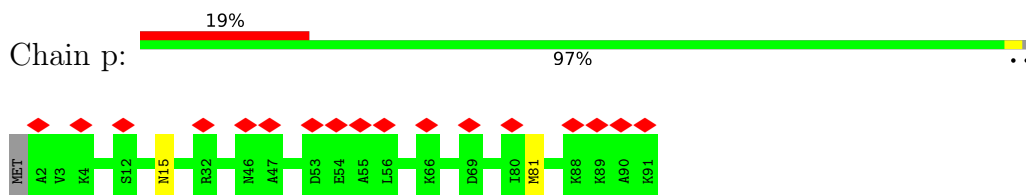
- Molecule 14: 30S ribosomal protein S14 type Z



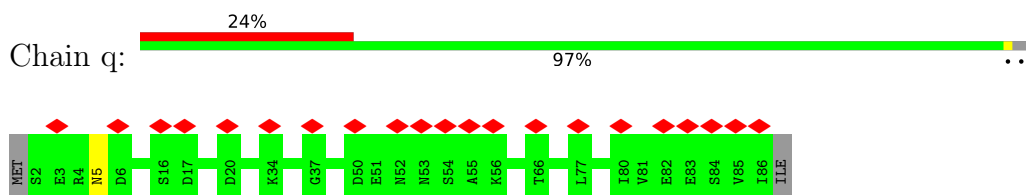
- Molecule 15: 30S ribosomal protein S15



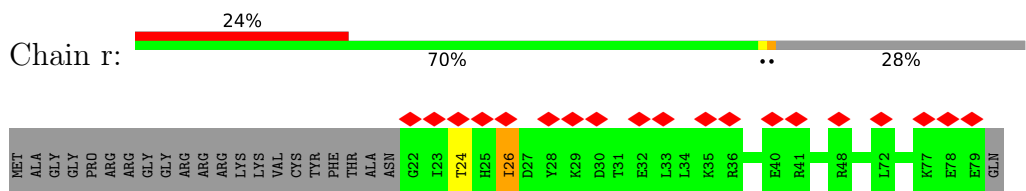
- Molecule 16: 30S ribosomal protein S16



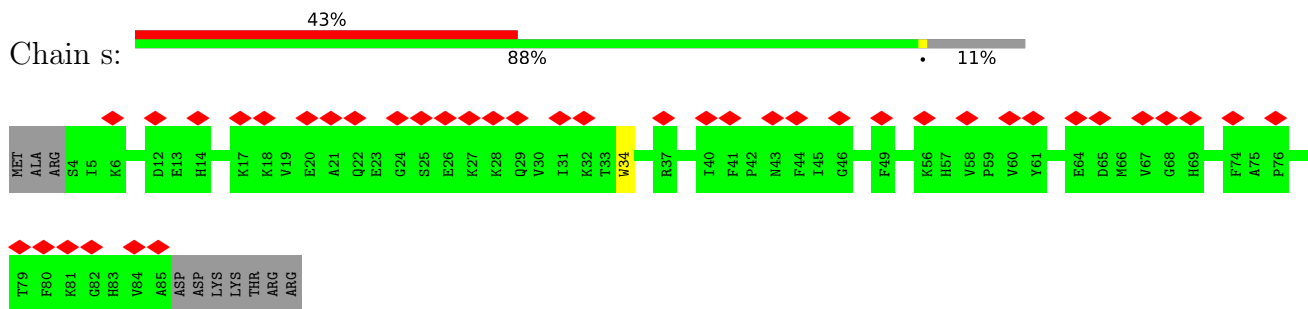
- Molecule 17: 30S ribosomal protein S17



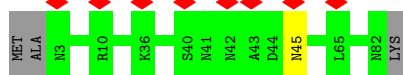
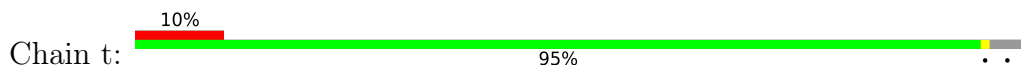
- Molecule 18: 30S ribosomal protein S18



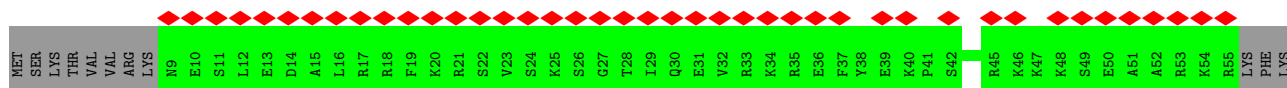
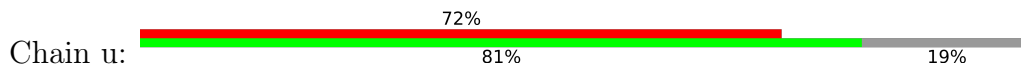
- Molecule 19: 30S ribosomal protein S19



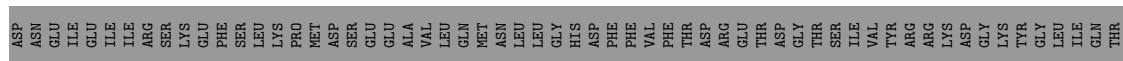
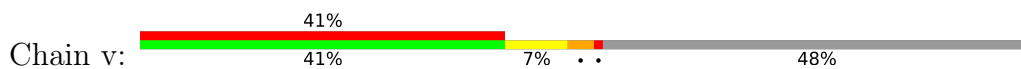
- Molecule 20: 30S ribosomal protein S20



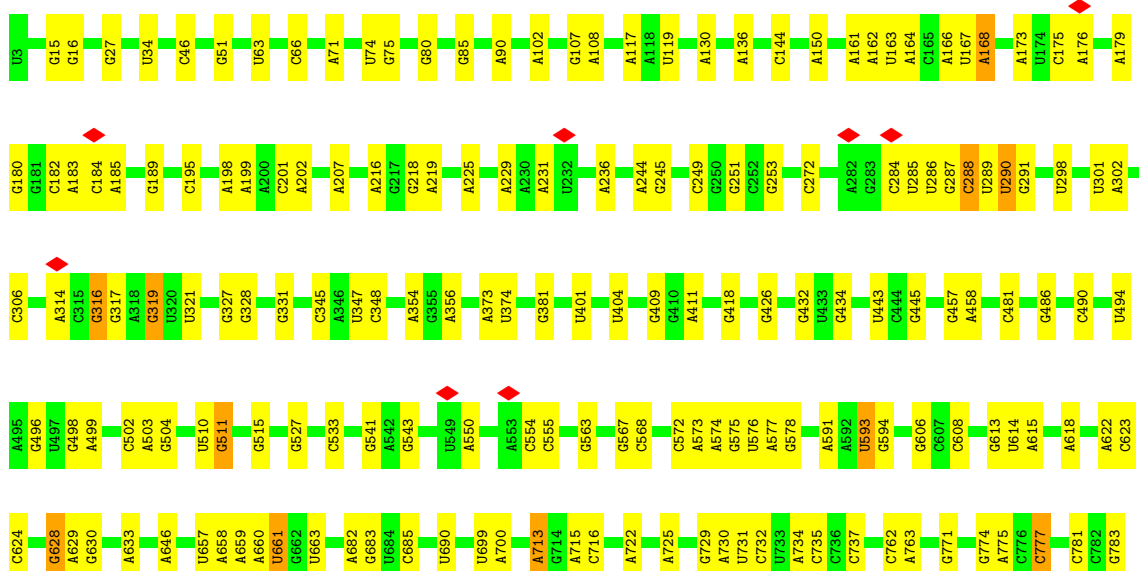
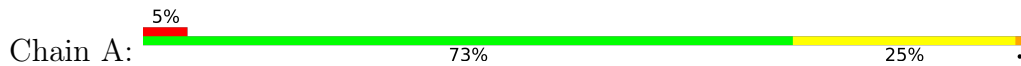
- Molecule 21: 30S ribosomal protein S21

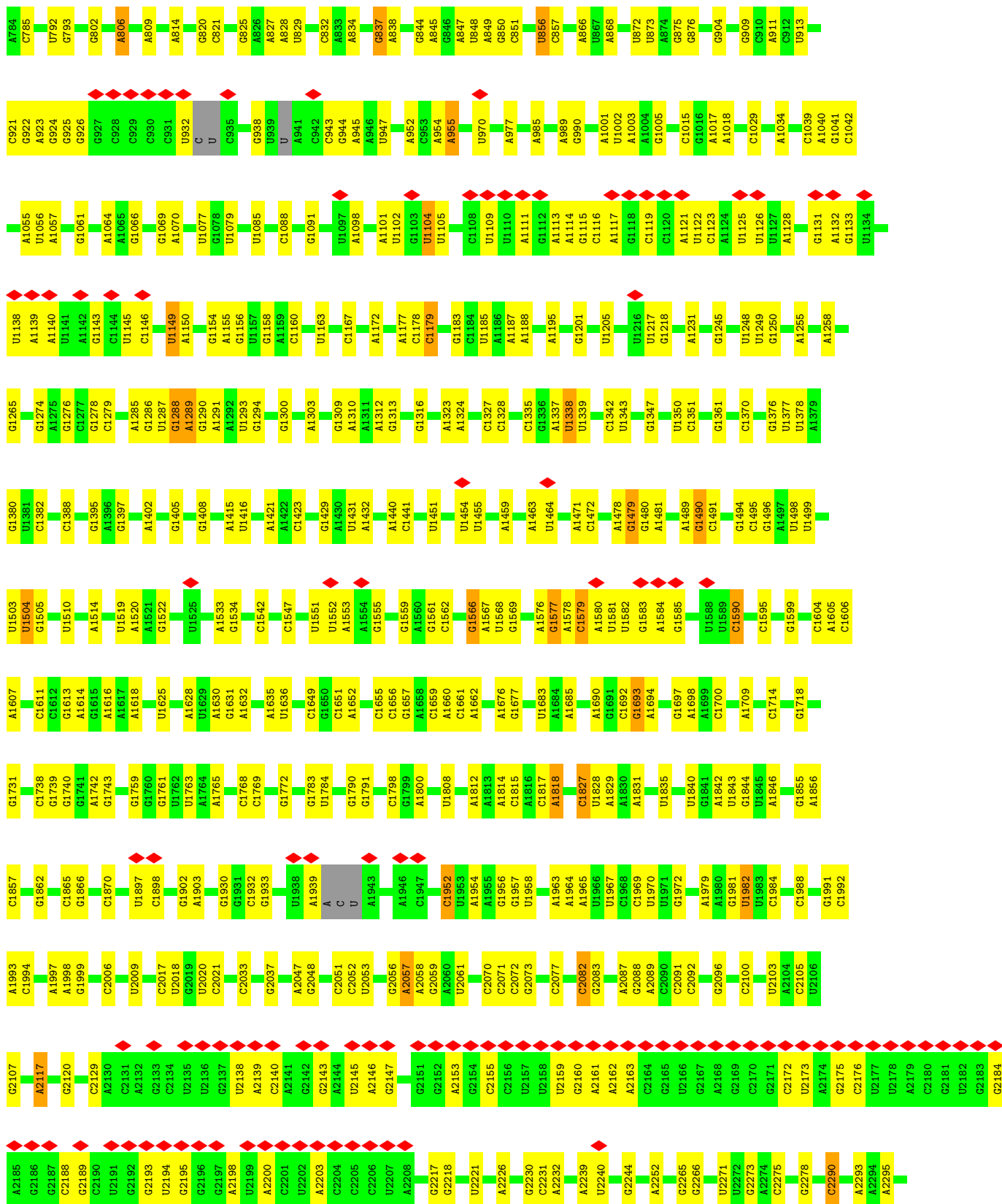


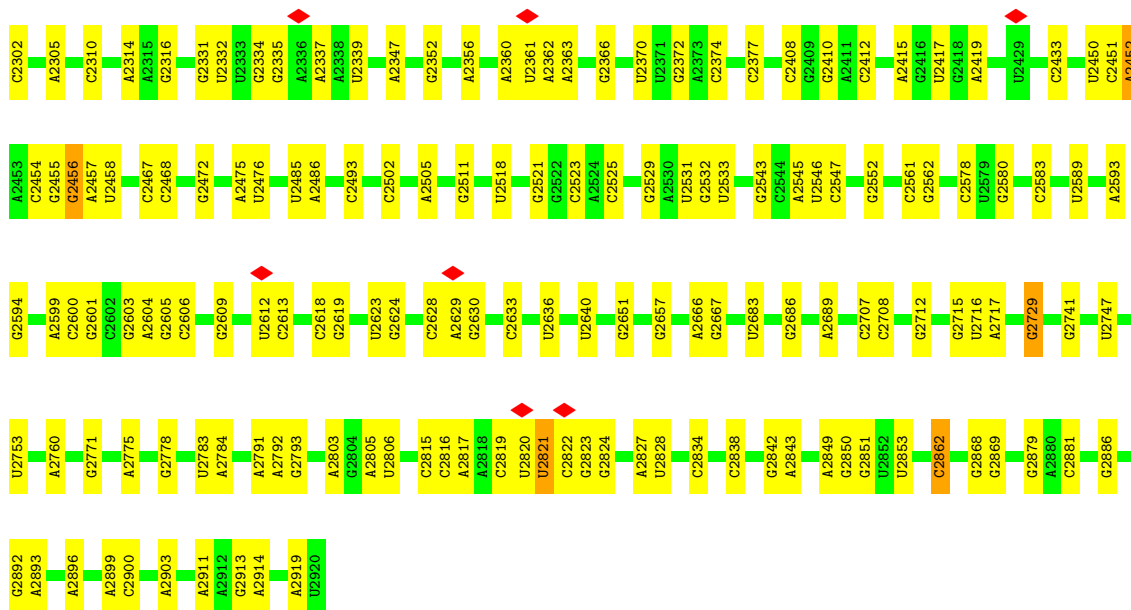
- Molecule 22: Ribosome hibernation promotion factor



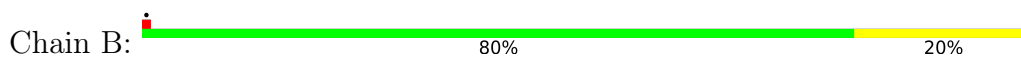
- Molecule 23: 23S ribosomal RNA



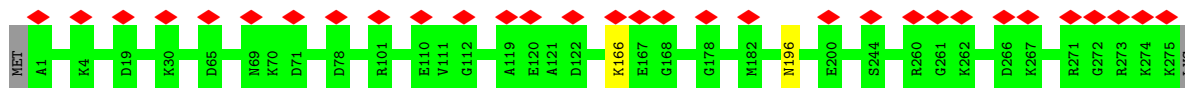




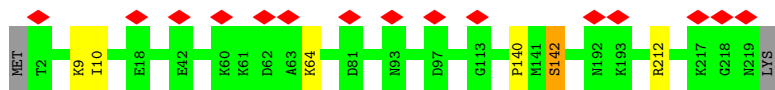
• Molecule 24: 5S ribosomal RNA



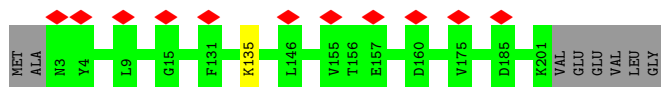
• Molecule 25: 50S ribosomal protein L2



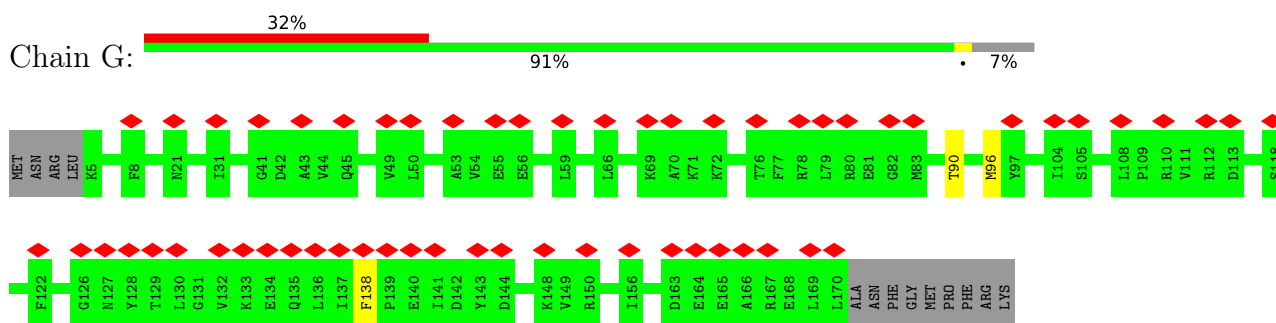
• Molecule 26: 50S ribosomal protein L3



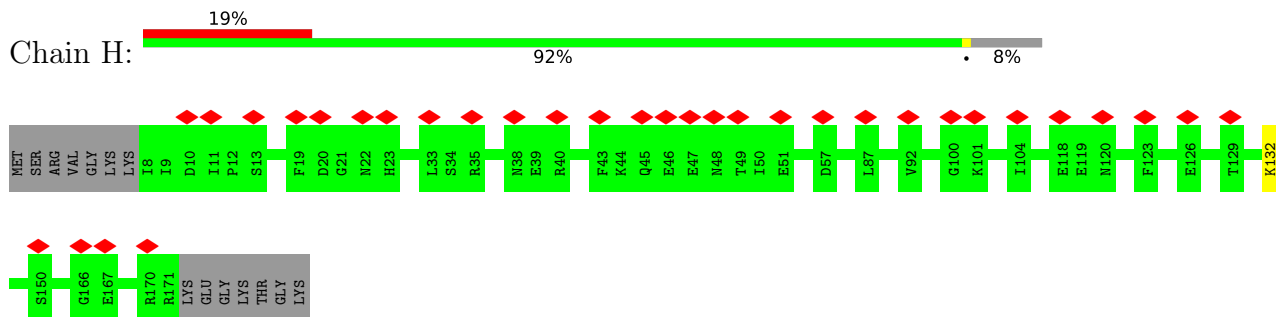
• Molecule 27: 50S ribosomal protein L4



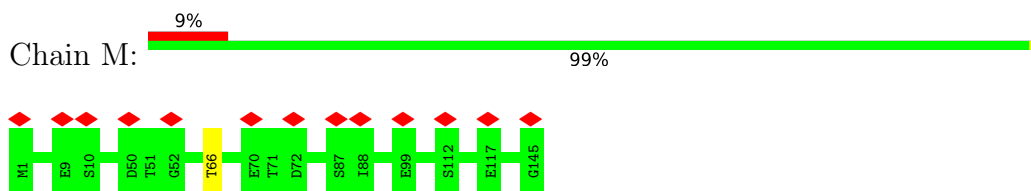
• Molecule 28: 50S ribosomal protein L5



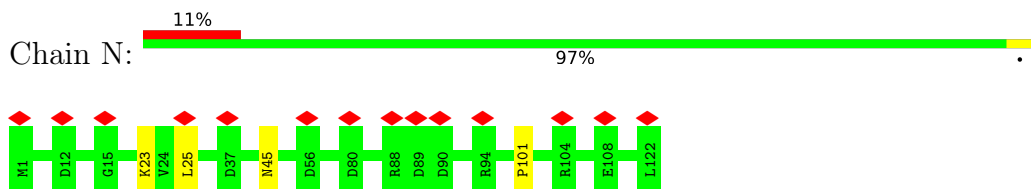
- Molecule 29: 50S ribosomal protein L6



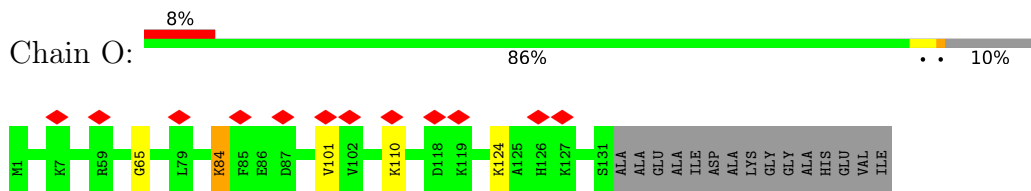
- Molecule 30: 50S ribosomal protein L13



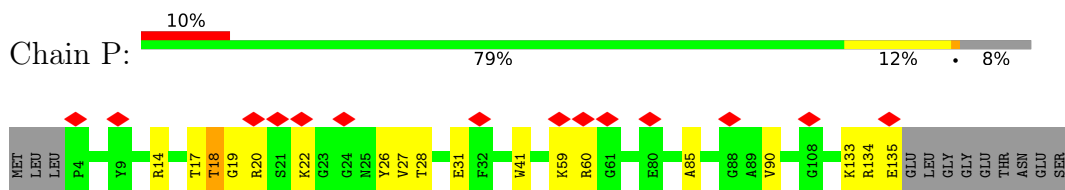
- Molecule 31: 50S ribosomal protein L14



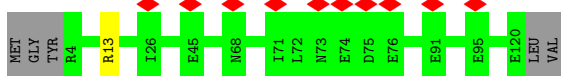
- Molecule 32: 50S ribosomal protein L15



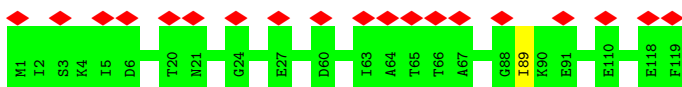
- Molecule 33: 50S ribosomal protein L16



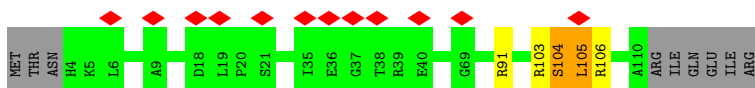
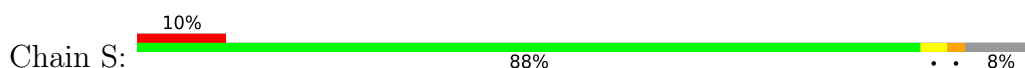
- Molecule 34: 50S ribosomal protein L17



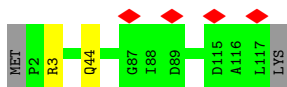
- Molecule 35: 50S ribosomal protein L18



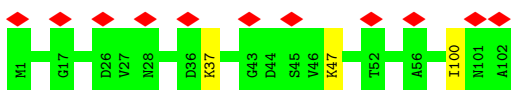
- Molecule 36: 50S ribosomal protein L19



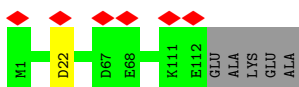
- Molecule 37: 50S ribosomal protein L20



- Molecule 38: 50S ribosomal protein L21



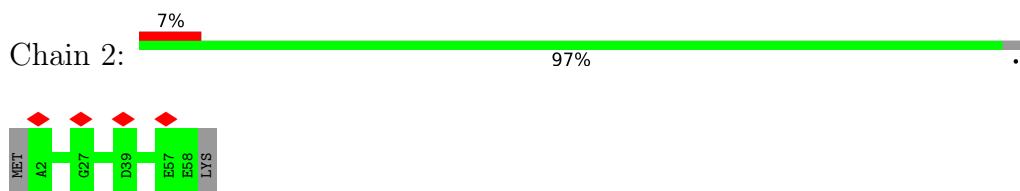
- Molecule 39: 50S ribosomal protein L22



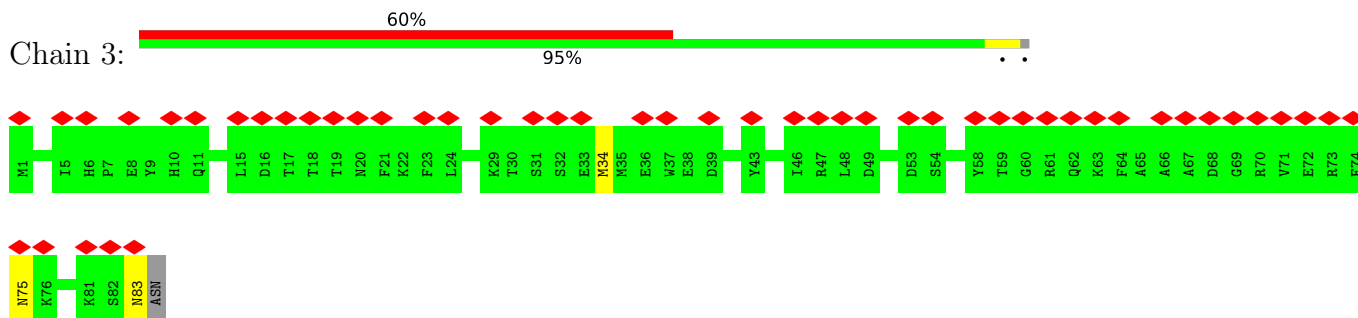
- Molecule 40: 50S ribosomal protein L23



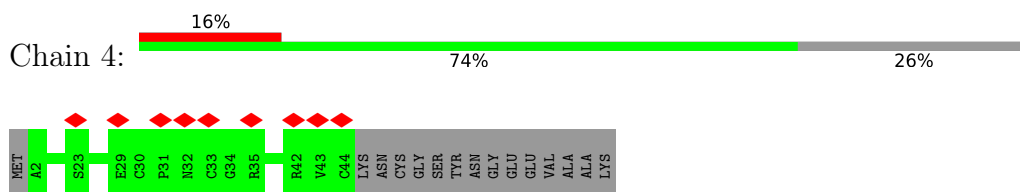
- Molecule 46: 50S ribosomal protein L30



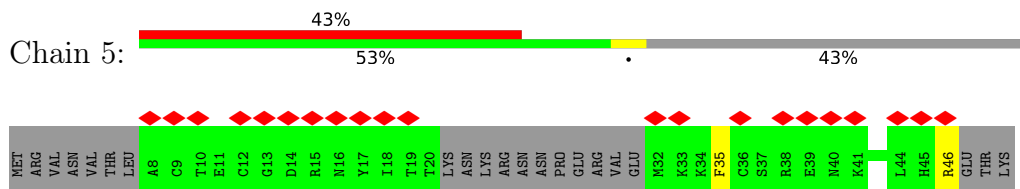
- Molecule 47: 50S ribosomal protein L31 type B



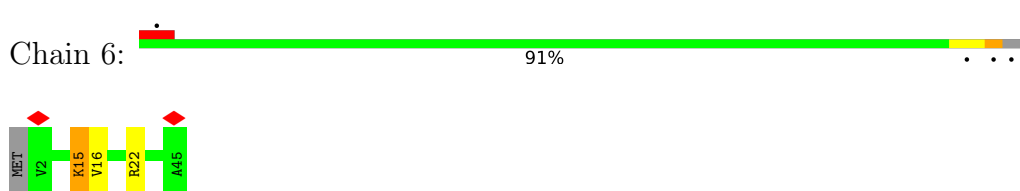
- Molecule 48: 50S ribosomal protein L32



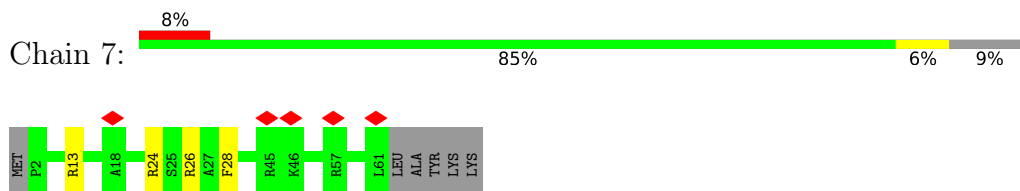
- Molecule 49: 50S ribosomal protein L33 2



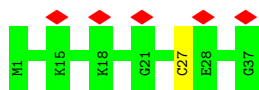
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	83000	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 ($e^-/\text{\AA}^2$)	60	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	0.253	Depositor
Minimum map value	-0.114	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	1.0, 1.0, 1.0	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.82	0/36976	1.11	76/57663 (0.1%)
2	b	0.40	0/1816	0.64	1/2436 (0.0%)
3	c	0.40	0/1631	0.71	1/2190 (0.0%)
4	d	0.42	0/1629	0.66	0/2185
5	e	0.43	0/1199	0.65	0/1616
6	f	0.48	0/792	0.68	0/1062
7	g	0.37	0/1157	0.66	0/1557
8	h	0.48	0/1044	0.73	2/1401 (0.1%)
9	i	0.38	0/1033	0.69	0/1386
10	j	0.41	0/803	0.71	2/1082 (0.2%)
11	k	0.37	0/895	0.66	0/1207
12	l	0.48	0/1075	0.72	0/1439
13	m	0.37	0/883	0.72	0/1182
14	n	0.47	0/512	0.84	1/678 (0.1%)
15	o	0.45	0/747	0.71	0/996
16	p	0.47	0/723	0.68	0/971
17	q	0.46	0/706	0.70	0/944
18	r	0.44	0/485	0.72	0/648
19	s	0.38	0/679	0.69	0/912
20	t	0.39	0/606	0.66	0/810
21	u	0.39	0/399	0.74	0/523
22	v	0.39	0/818	0.90	5/1101 (0.5%)
23	A	1.12	14/69927 (0.0%)	1.25	306/109056 (0.3%)
24	B	0.84	0/2717	1.19	13/4232 (0.3%)
25	D	0.66	0/2138	0.73	0/2869
26	E	0.62	0/1673	0.69	0/2243
27	F	0.57	0/1547	0.67	0/2088
28	G	0.43	0/1326	0.70	0/1780
29	H	0.41	0/1302	0.64	0/1757
30	M	0.57	0/1173	0.69	0/1578
31	N	0.62	0/927	0.75	0/1243
32	O	0.55	0/1010	0.77	0/1344
33	P	0.59	0/1080	0.73	1/1448 (0.1%)
34	Q	0.54	0/927	0.71	1/1238 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	R	0.43	0/931	0.69	0/1244
36	S	0.60	0/874	0.82	1/1168 (0.1%)
37	T	0.70	0/955	0.76	1/1265 (0.1%)
38	U	0.61	0/809	0.70	0/1080
39	V	0.61	0/870	0.76	1/1171 (0.1%)
40	W	0.59	1/733 (0.1%)	0.68	0/978
41	X	0.51	0/672	0.68	0/893
42	Y	0.37	0/746	0.71	0/1000
43	Z	0.66	1/591 (0.2%)	0.63	0/785
44	0	0.48	0/378	0.77	0/504
45	1	0.44	0/537	0.64	0/714
46	2	0.53	0/443	0.73	0/597
47	3	0.42	0/694	0.69	0/930
48	4	0.59	0/357	0.70	0/474
49	5	0.37	0/230	0.73	0/303
50	6	0.76	0/377	0.87	2/491 (0.4%)
51	7	0.60	0/491	0.85	1/643 (0.2%)
52	8	0.57	0/300	0.71	0/393
All	All	0.90	16/153343 (0.0%)	1.10	415/229498 (0.2%)

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
2	b	0	1
3	c	0	1
4	d	0	2
6	f	0	1
7	g	0	1
12	l	0	1
13	m	0	1
14	n	0	2
17	q	0	1
18	r	0	1
19	s	0	1
22	v	0	8
25	D	0	1
26	E	0	3
28	G	0	1
31	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	O	0	4
33	P	0	3
35	R	0	1
36	S	0	3
38	U	0	2
40	W	0	1
41	X	0	1
45	1	0	1
50	6	0	1
51	7	0	2
52	8	0	1
All	All	0	47

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	1289	A	C6-N6	-6.70	1.28	1.33
40	W	58	TYR	C-N	-5.96	1.20	1.34
23	A	2091	C	C4-C5	-5.63	1.38	1.43
23	A	2604	A	N9-C4	-5.58	1.34	1.37
23	A	511	G	N9-C8	-5.56	1.33	1.37

The worst 5 of 415 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	624	C	N3-C2-O2	-10.48	114.56	121.90
23	A	623	C	N1-C2-O2	9.90	124.84	118.90
23	A	2451	C	N3-C2-O2	-9.69	115.12	121.90
23	A	624	C	C6-N1-C2	-9.58	116.47	120.30
23	A	2451	C	C2-N1-C1'	9.45	129.19	118.80

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	b	94	GLN	Peptide
3	c	160	ASP	Peptide
4	d	198	TYR	Peptide
4	d	44	LEU	Peptide
6	f	68	ASP	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	
2	b	220/255 (86%)	186 (84%)	34 (16%)	0	100	100
3	c	202/217 (93%)	173 (86%)	29 (14%)	0	100	100
4	d	193/200 (96%)	169 (88%)	24 (12%)	0	100	100
5	e	157/166 (95%)	134 (85%)	23 (15%)	0	100	100
6	f	92/98 (94%)	77 (84%)	15 (16%)	0	100	100
7	g	139/156 (89%)	115 (83%)	22 (16%)	2 (1%)	11	45
8	h	129/132 (98%)	107 (83%)	21 (16%)	1 (1%)	19	56
9	i	126/132 (96%)	115 (91%)	11 (9%)	0	100	100
10	j	97/102 (95%)	81 (84%)	16 (16%)	0	100	100
11	k	116/129 (90%)	100 (86%)	16 (14%)	0	100	100
12	l	133/137 (97%)	109 (82%)	23 (17%)	1 (1%)	19	56
13	m	108/121 (89%)	94 (87%)	13 (12%)	1 (1%)	17	54
14	n	58/61 (95%)	45 (78%)	13 (22%)	0	100	100
15	o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
16	p	88/91 (97%)	70 (80%)	18 (20%)	0	100	100
17	q	83/87 (95%)	63 (76%)	20 (24%)	0	100	100
18	r	56/80 (70%)	53 (95%)	3 (5%)	0	100	100
19	s	80/92 (87%)	60 (75%)	20 (25%)	0	100	100
20	t	78/83 (94%)	68 (87%)	10 (13%)	0	100	100
21	u	45/58 (78%)	45 (100%)	0	0	100	100
22	v	96/190 (50%)	74 (77%)	16 (17%)	6 (6%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	D	273/277 (99%)	228 (84%)	45 (16%)	0	100	100
26	E	216/220 (98%)	171 (79%)	43 (20%)	2 (1%)	17	54
27	F	197/207 (95%)	150 (76%)	47 (24%)	0	100	100
28	G	164/179 (92%)	121 (74%)	42 (26%)	1 (1%)	25	62
29	H	162/178 (91%)	138 (85%)	24 (15%)	0	100	100
30	M	143/145 (99%)	119 (83%)	23 (16%)	1 (1%)	22	59
31	N	120/122 (98%)	95 (79%)	23 (19%)	2 (2%)	9	42
32	O	129/146 (88%)	93 (72%)	36 (28%)	0	100	100
33	P	130/144 (90%)	96 (74%)	31 (24%)	3 (2%)	6	36
34	Q	115/122 (94%)	94 (82%)	21 (18%)	0	100	100
35	R	117/119 (98%)	95 (81%)	22 (19%)	0	100	100
36	S	105/116 (90%)	86 (82%)	16 (15%)	3 (3%)	4	32
37	T	114/118 (97%)	100 (88%)	14 (12%)	0	100	100
38	U	100/102 (98%)	86 (86%)	14 (14%)	0	100	100
39	V	110/117 (94%)	100 (91%)	10 (9%)	0	100	100
40	W	87/91 (96%)	64 (74%)	23 (26%)	0	100	100
41	X	81/105 (77%)	59 (73%)	21 (26%)	1 (1%)	13	48
42	Y	92/217 (42%)	65 (71%)	26 (28%)	1 (1%)	14	50
43	Z	74/94 (79%)	53 (72%)	19 (26%)	2 (3%)	5	33
44	0	44/62 (71%)	32 (73%)	12 (27%)	0	100	100
45	1	63/69 (91%)	60 (95%)	3 (5%)	0	100	100
46	2	55/59 (93%)	49 (89%)	6 (11%)	0	100	100
47	3	81/84 (96%)	62 (76%)	18 (22%)	1 (1%)	13	48
48	4	41/58 (71%)	36 (88%)	5 (12%)	0	100	100
49	5	24/49 (49%)	16 (67%)	8 (33%)	0	100	100
50	6	42/45 (93%)	35 (83%)	5 (12%)	2 (5%)	2	22
51	7	58/66 (88%)	44 (76%)	14 (24%)	0	100	100
52	8	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
All	All	5354/6024 (89%)	4397 (82%)	927 (17%)	30 (1%)	29	62

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	v	6	ILE
22	v	51	ALA
22	v	69	GLU
22	v	93	LYS
26	E	10	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	192/221 (87%)	191 (100%)	1 (0%)	88	94
3	c	165/175 (94%)	161 (98%)	4 (2%)	49	71
4	d	172/175 (98%)	171 (99%)	1 (1%)	86	93
5	e	125/131 (95%)	123 (98%)	2 (2%)	62	80
6	f	82/86 (95%)	81 (99%)	1 (1%)	71	84
7	g	122/132 (92%)	118 (97%)	4 (3%)	38	64
8	h	112/113 (99%)	111 (99%)	1 (1%)	78	88
9	i	106/109 (97%)	106 (100%)	0	100	100
10	j	89/91 (98%)	89 (100%)	0	100	100
11	k	94/104 (90%)	94 (100%)	0	100	100
12	l	117/119 (98%)	116 (99%)	1 (1%)	78	88
13	m	94/104 (90%)	93 (99%)	1 (1%)	73	85
14	n	52/53 (98%)	51 (98%)	1 (2%)	57	76
15	o	80/81 (99%)	79 (99%)	1 (1%)	69	83
16	p	76/77 (99%)	74 (97%)	2 (3%)	46	69
17	q	80/82 (98%)	80 (100%)	0	100	100
18	r	52/68 (76%)	50 (96%)	2 (4%)	33	61
19	s	71/80 (89%)	71 (100%)	0	100	100
20	t	67/69 (97%)	66 (98%)	1 (2%)	65	81
21	u	43/54 (80%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	v	89/173 (51%)	80 (90%)	9 (10%)	7	31
25	D	222/224 (99%)	221 (100%)	1 (0%)	88	94
26	E	175/177 (99%)	173 (99%)	2 (1%)	73	85
27	F	163/169 (96%)	162 (99%)	1 (1%)	86	93
28	G	147/158 (93%)	146 (99%)	1 (1%)	84	91
29	H	144/155 (93%)	143 (99%)	1 (1%)	84	91
30	M	123/123 (100%)	123 (100%)	0	100	100
31	N	100/100 (100%)	99 (99%)	1 (1%)	76	86
32	O	104/112 (93%)	102 (98%)	2 (2%)	57	76
33	P	109/119 (92%)	97 (89%)	12 (11%)	6	29
34	Q	98/102 (96%)	98 (100%)	0	100	100
35	R	95/95 (100%)	95 (100%)	0	100	100
36	S	93/102 (91%)	93 (100%)	0	100	100
37	T	96/98 (98%)	95 (99%)	1 (1%)	76	86
38	U	86/86 (100%)	85 (99%)	1 (1%)	71	84
39	V	91/94 (97%)	91 (100%)	0	100	100
40	W	80/82 (98%)	79 (99%)	1 (1%)	69	83
41	X	73/90 (81%)	73 (100%)	0	100	100
42	Y	83/190 (44%)	83 (100%)	0	100	100
43	Z	59/75 (79%)	50 (85%)	9 (15%)	2	17
44	0	39/52 (75%)	37 (95%)	2 (5%)	24	55
45	1	59/62 (95%)	59 (100%)	0	100	100
46	2	51/53 (96%)	51 (100%)	0	100	100
47	3	74/75 (99%)	72 (97%)	2 (3%)	44	68
48	4	40/51 (78%)	40 (100%)	0	100	100
49	5	26/47 (55%)	24 (92%)	2 (8%)	13	43
50	6	39/40 (98%)	39 (100%)	0	100	100
51	7	52/57 (91%)	51 (98%)	1 (2%)	57	76
52	8	35/35 (100%)	35 (100%)	0	100	100
All	All	4636/5120 (90%)	4564 (98%)	72 (2%)	64	80

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	Z	20	ASN
51	7	26	ARG
43	Z	23	ASP
44	0	23	ASN
22	v	5	GLU

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

Mol	Chain	Res	Type
29	H	38	ASN
38	U	63	ASN
29	H	74	ASN
31	N	45	ASN
39	V	102	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1541/1547 (99%)	303 (19%)	0
23	A	2907/2918 (99%)	625 (21%)	8 (0%)
24	B	113/114 (99%)	18 (15%)	0
All	All	4561/4579 (99%)	946 (20%)	8 (0%)

5 of 946 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	8	G
1	a	9	A
1	a	10	G
1	a	11	A
1	a	17	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	A	2715	G
23	A	2056	G
23	A	1478	A
23	A	1288	G
23	A	1982	U

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
23	A	1
40	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1569:G	O3'	1570:G	P	3.93
1	W	58:TYR	C	59:LYS	N	1.20

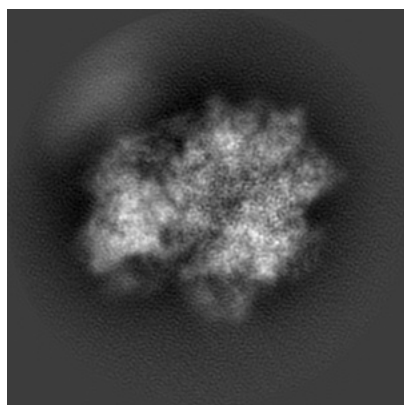
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3624. These allow visual inspection of the internal detail of the map and identification of artifacts.

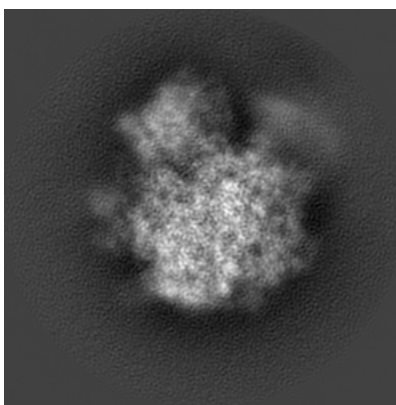
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

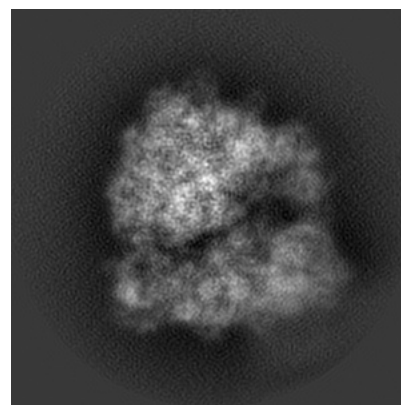
6.1.1 Primary map



X



Y

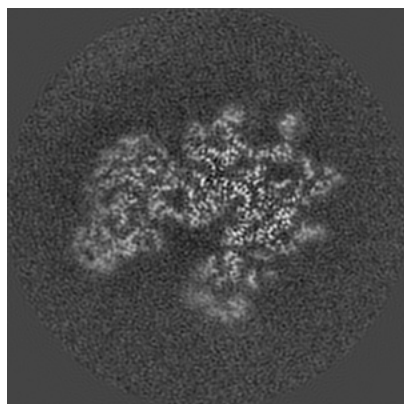


Z

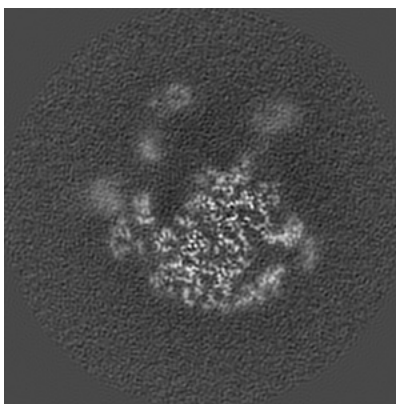
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

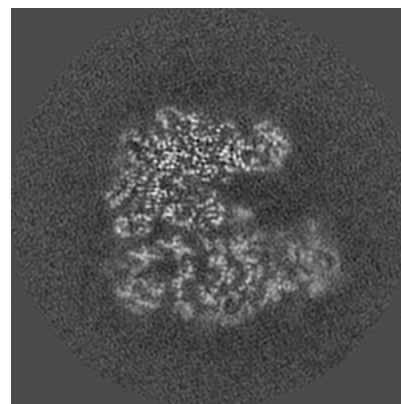
6.2.1 Primary map



X Index: 170



Y Index: 170

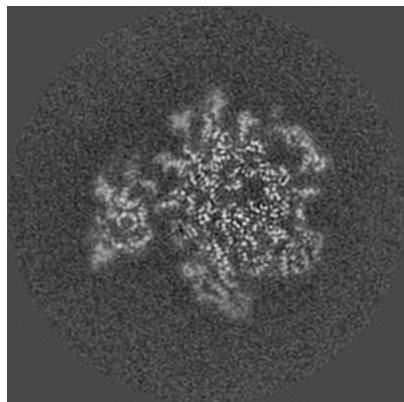


Z Index: 170

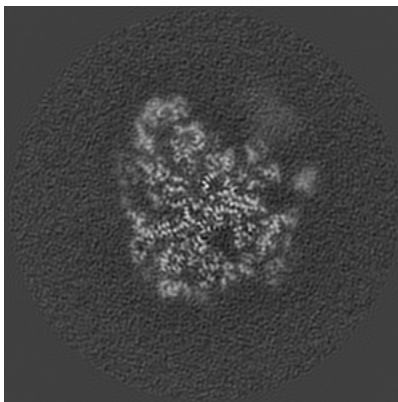
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

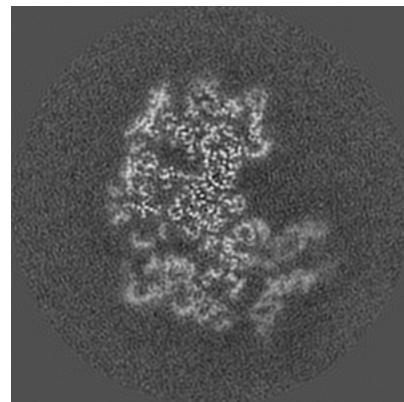
6.3.1 Primary map



X Index: 142



Y Index: 213



Z Index: 189

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

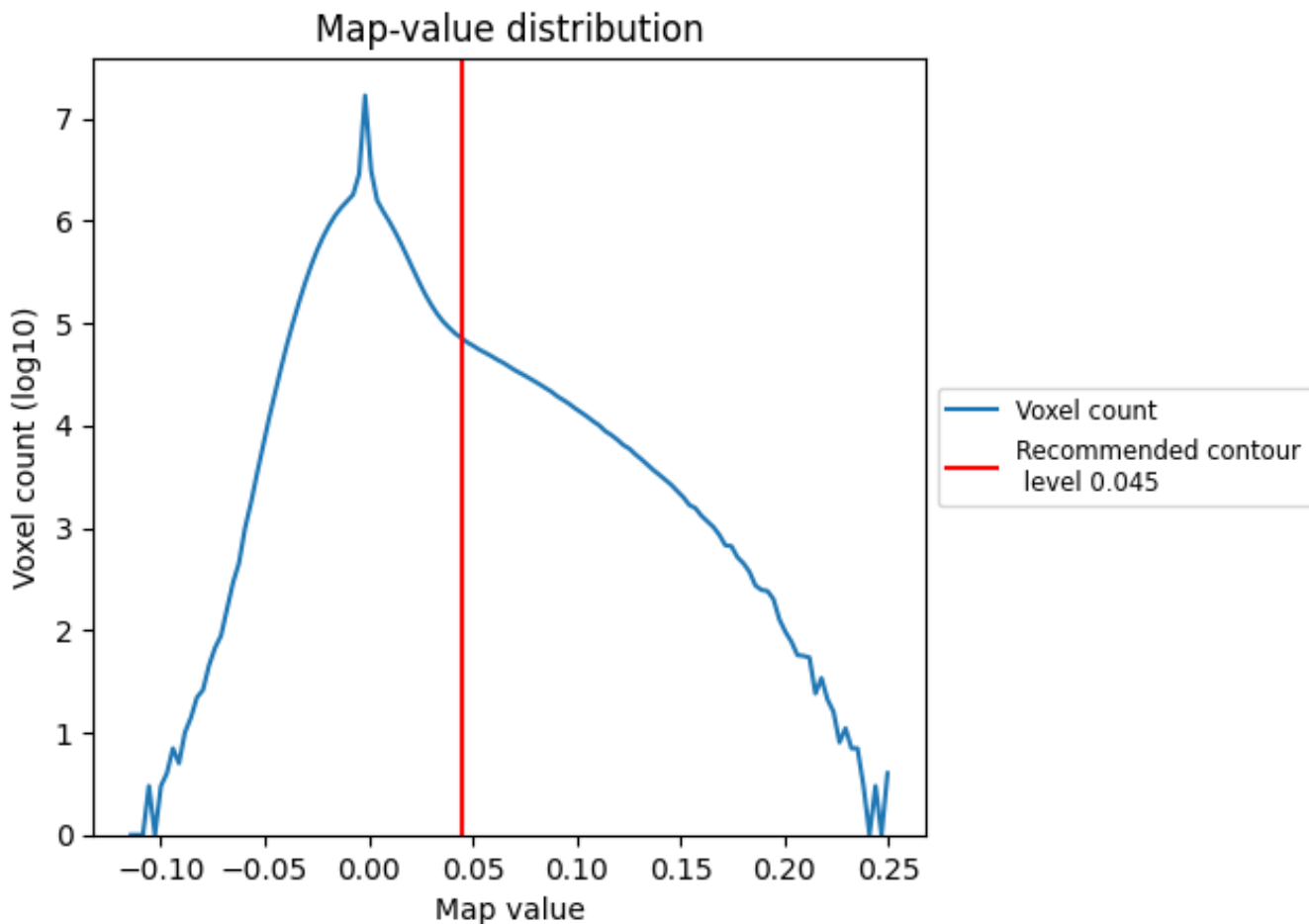
6.5 Mask visualisation

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

7 Map analysis [i](#)

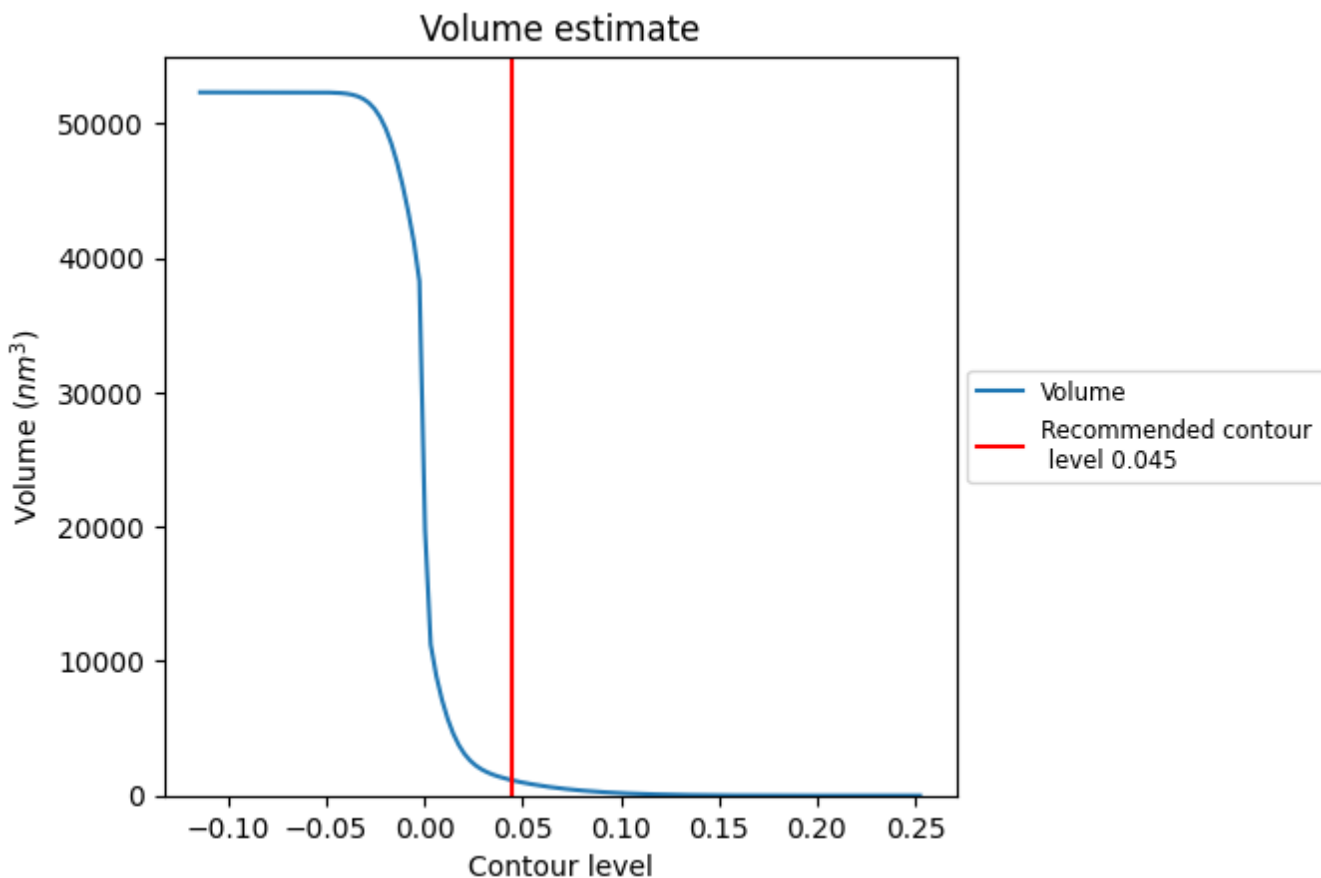
This section contains the results of statistical analysis of the map.

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.

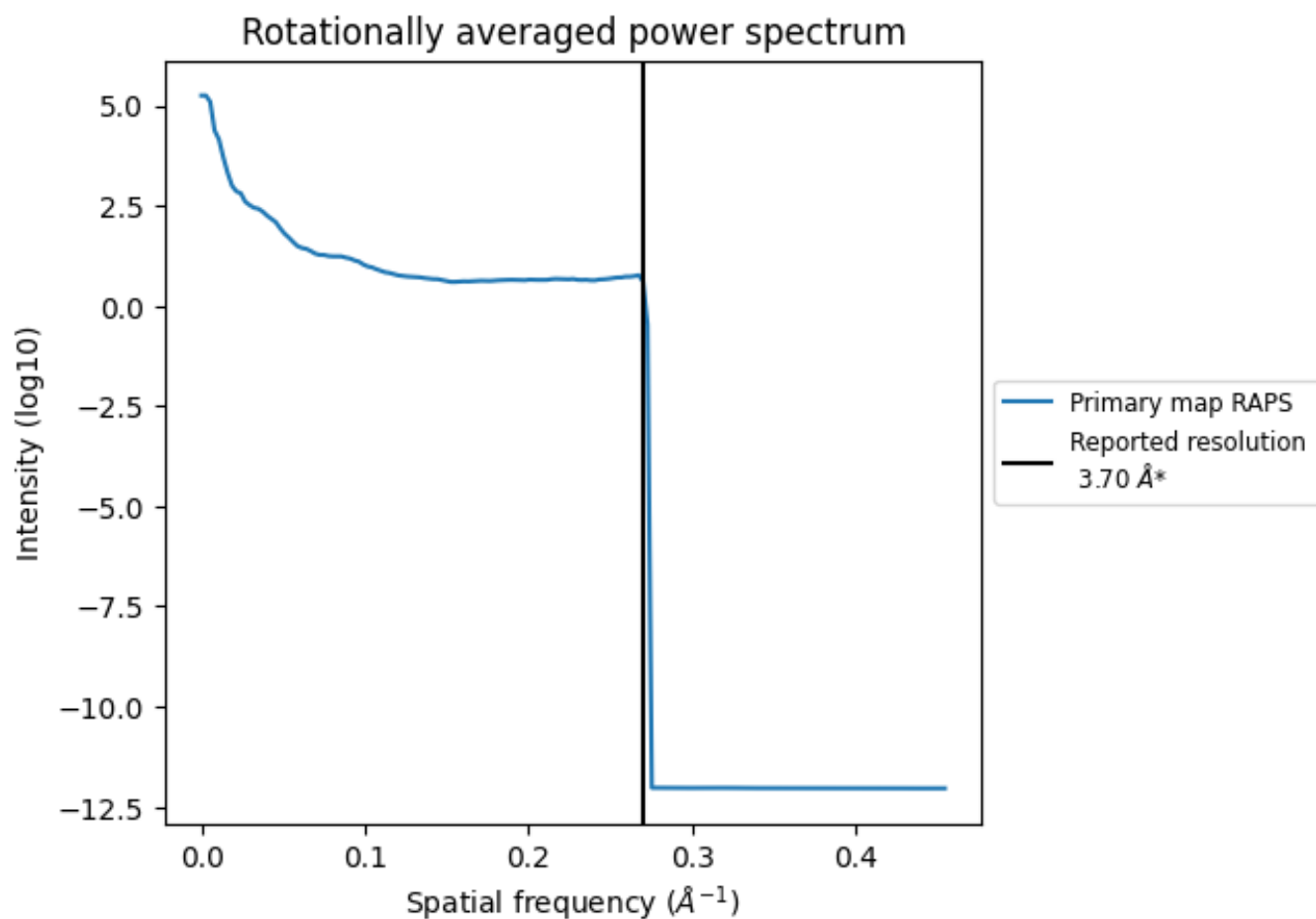
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1129 nm³; this corresponds to an approximate mass of 1020 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 0.270 Å⁻¹

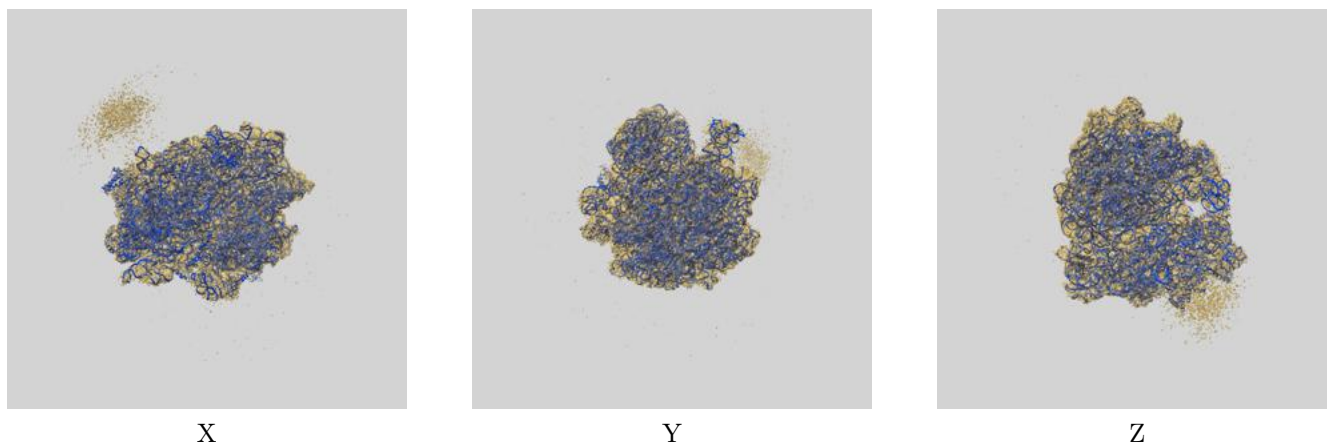
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

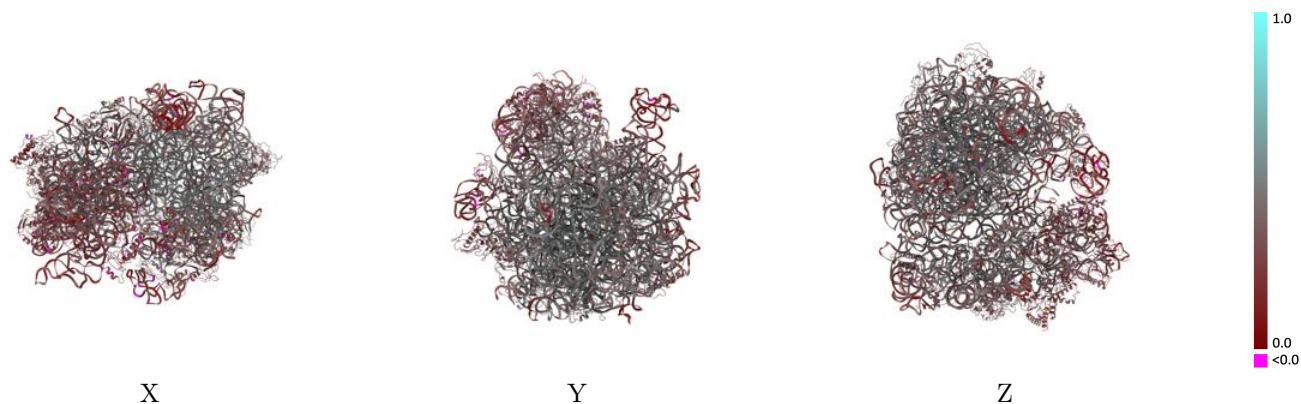
This section contains information regarding the fit between EMDB map EMD-3624 and PDB model 5ND8. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



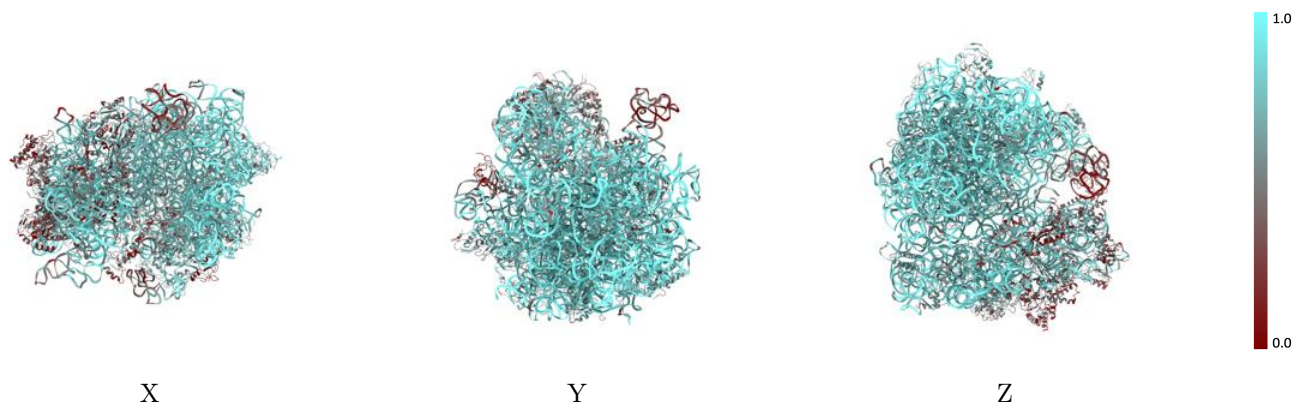
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



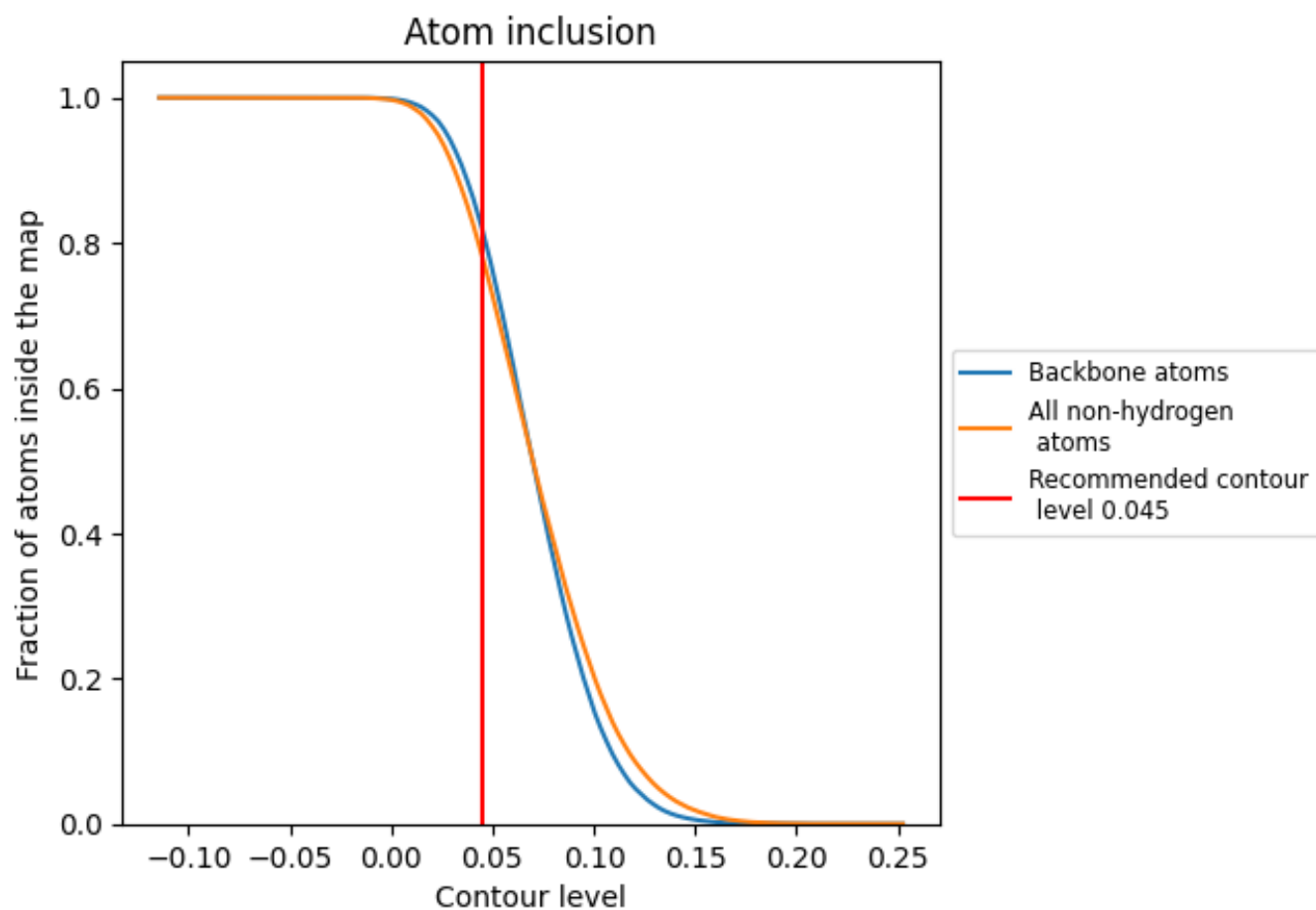
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 78% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7816	 0.3840
0	 0.5938	 0.3890
1	 0.6558	 0.3660
2	 0.6905	 0.4250
3	 0.3338	 0.1880
4	 0.6220	 0.4270
5	 0.2703	 0.2780
6	 0.7500	 0.4580
7	 0.7164	 0.4150
8	 0.6564	 0.4350
A	 0.8907	 0.4180
B	 0.9156	 0.3550
D	 0.6898	 0.4560
E	 0.7083	 0.4370
F	 0.6973	 0.4010
G	 0.5128	 0.2740
H	 0.5876	 0.3120
M	 0.7177	 0.4260
N	 0.6310	 0.4420
O	 0.7115	 0.3960
P	 0.6807	 0.3890
Q	 0.6928	 0.4180
R	 0.6300	 0.3130
S	 0.6606	 0.4230
T	 0.7462	 0.4280
U	 0.6925	 0.4290
V	 0.7155	 0.4610
W	 0.6634	 0.4070
X	 0.6369	 0.3690
Y	 0.2152	 0.3000
Z	 0.7420	 0.4350
a	 0.8631	 0.3590
b	 0.3210	 0.2990
c	 0.2734	 0.2950
d	 0.4839	 0.2820



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Chain	Atom inclusion	Q-score
e	 0.5056	 0.3720
f	 0.4373	 0.3500
g	 0.4081	 0.2700
h	 0.5669	 0.3590
i	 0.3432	 0.2470
j	 0.2902	 0.2630
k	 0.4611	 0.3280
l	 0.5965	 0.3860
m	 0.3722	 0.2240
n	 0.3825	 0.2700
o	 0.6107	 0.3480
p	 0.5986	 0.3520
q	 0.5653	 0.3710
r	 0.4989	 0.3840
s	 0.3954	 0.2130
t	 0.6388	 0.3320
u	 0.1557	 0.2810
v	 0.2255	 0.2870