



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 04:26 AM UTC

PDB ID : 6HA8 / pdb_00006ha8
EMDB ID : EMD-0177
Title : Cryo-EM structure of the ABCF protein VmlR bound to the Bacillus subtilis ribosome
Authors : Crowe-McAuliffe, C.; Graf, M.; Huter, P.; Abdelshahid, M.; Novacek, J.; Wilson, D.N.
Deposited on : 2018-08-07
Resolution : 3.50 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:

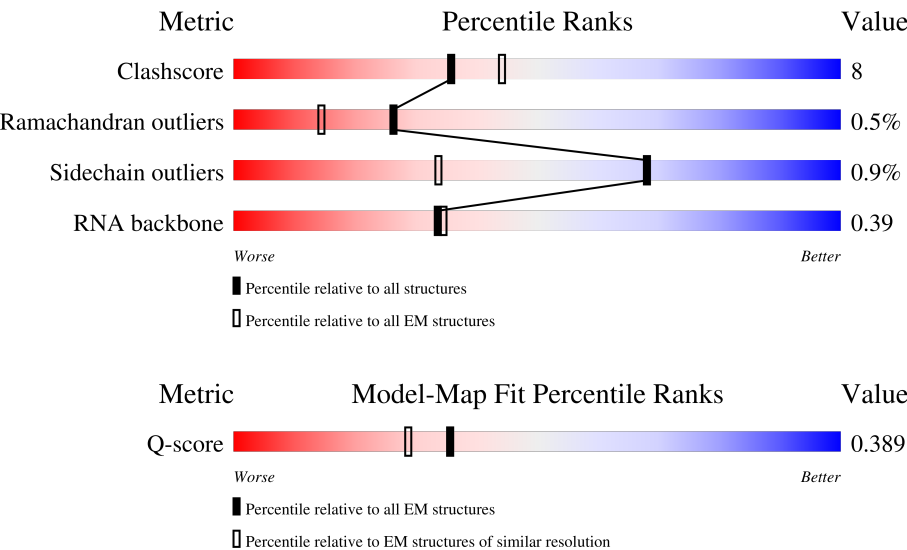
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.50 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.



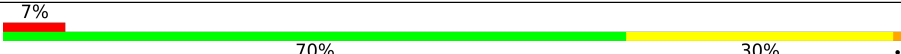
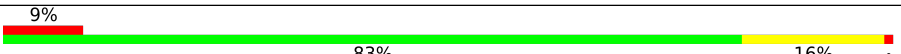
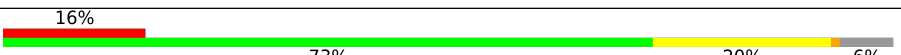
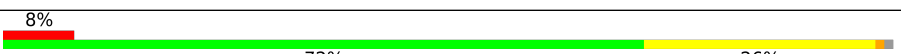
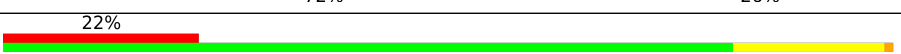
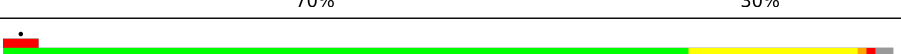
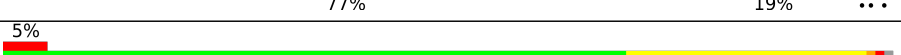
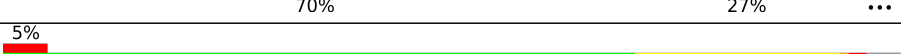
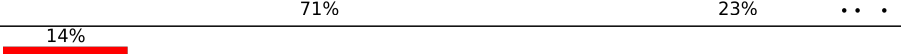
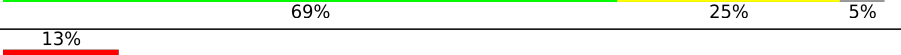
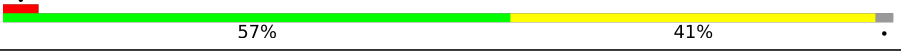
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	2928	
2	B	112	
3	C	277	

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Mol	Chain	Length	Quality of chain
4	D	209	
5	E	207	
6	F	179	
7	G	179	
8	J	145	
9	K	122	
10	L	146	
11	M	144	
12	N	120	
13	O	120	
14	P	115	
15	Q	119	
16	R	102	
17	S	113	
18	T	95	
19	U	103	
20	V	548	
21	W	94	
22	X	62	
23	Y	66	
24	Z	59	
25	0	59	
26	1	49	
27	2	44	
28	3	66	

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Mol	Chain	Length	Quality of chain
29	4	37	
30	6	66	
31	7	3	
32	8	232	
33	a	1554	
34	b	246	
35	c	218	
36	d	200	
37	e	166	
38	f	95	
39	g	156	
40	h	132	
41	i	130	
42	j	102	
43	k	131	
44	l	138	
45	m	121	
46	n	61	
47	o	89	
48	p	90	
49	q	87	
50	r	79	
51	s	92	
52	t	88	
53	x	75	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	TEL	A	3001	X	-	-	-
55	ATP	V	900	-	-	X	-
55	ATP	V	901	-	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 146404 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2887	Total	C	N	O	P	0	0
			61997	27661	11460	19992	2884		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	176	Total	C	N	O	S	0	0
			1386	882	241	256	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	146	Total	C	N	O	S	0	0
			1081	671	207	201	2		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	120	Total	C	N	O	S	0	0
			912	564	176	171	1		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	115	Total	C	N	O	S	0	0
			944	600	185	158	1		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	101	Total	C	N	O		0	0
			786	501	139	146			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

- Molecule 20 is a protein called Nucleotide-binding protein ExpZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	541	Total	C	N	O	S	0	0
			4177	2637	737	796	7		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-5	MET	-	initiating methionine	UNP P39115
V	-4	HIS	-	expression tag	UNP P39115
V	-3	HIS	-	expression tag	UNP P39115
V	-2	HIS	-	expression tag	UNP P39115
V	-1	HIS	-	expression tag	UNP P39115
V	0	HIS	-	expression tag	UNP P39115
V	1	HIS	-	expression tag	UNP P39115
V	129	GLN	GLU	engineered mutation	UNP P39115
V	432	GLN	GLU	engineered mutation	UNP P39115
V	486	ALA	-	expression tag	UNP P39115
V	487	ALA	-	expression tag	UNP P39115
V	488	ALA	-	expression tag	UNP P39115
V	489	ALA	-	expression tag	UNP P39115
V	490	ALA	-	expression tag	UNP P39115
V	491	ALA	-	expression tag	UNP P39115
V	492	ALA	-	expression tag	UNP P39115
V	493	ALA	-	expression tag	UNP P39115
V	494	ALA	-	expression tag	UNP P39115
V	495	ALA	-	expression tag	UNP P39115
V	496	ALA	-	expression tag	UNP P39115
V	497	ALA	-	expression tag	UNP P39115
V	498	ALA	-	expression tag	UNP P39115
V	499	ALA	-	expression tag	UNP P39115
V	500	ALA	-	expression tag	UNP P39115
V	501	ALA	-	expression tag	UNP P39115
V	502	ALA	-	expression tag	UNP P39115
V	503	ALA	-	expression tag	UNP P39115
V	504	ALA	-	expression tag	UNP P39115
V	505	ALA	-	expression tag	UNP P39115
V	506	ALA	-	expression tag	UNP P39115
V	507	ALA	-	expression tag	UNP P39115
V	508	ALA	-	expression tag	UNP P39115
V	509	ALA	-	expression tag	UNP P39115
V	510	ALA	-	expression tag	UNP P39115
V	511	ALA	-	expression tag	UNP P39115
V	512	ALA	-	expression tag	UNP P39115
V	513	ALA	-	expression tag	UNP P39115
V	514	ALA	-	expression tag	UNP P39115
V	515	ALA	-	expression tag	UNP P39115
V	516	ALA	-	expression tag	UNP P39115
V	517	ALA	-	expression tag	UNP P39115
V	518	ALA	-	expression tag	UNP P39115
V	519	ALA	-	expression tag	UNP P39115

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Chain	Residue	Modelled	Actual	Comment	Reference
V	520	ALA	-	expression tag	UNP P39115
V	521	ALA	-	expression tag	UNP P39115
V	522	ALA	-	expression tag	UNP P39115
V	523	ALA	-	expression tag	UNP P39115
V	524	ALA	-	expression tag	UNP P39115
V	525	ALA	-	expression tag	UNP P39115
V	526	ALA	-	expression tag	UNP P39115
V	527	ALA	-	expression tag	UNP P39115
V	528	ALA	-	expression tag	UNP P39115
V	529	ALA	-	expression tag	UNP P39115
V	530	ALA	-	expression tag	UNP P39115
V	531	ALA	-	expression tag	UNP P39115
V	532	ALA	-	expression tag	UNP P39115
V	533	ALA	-	expression tag	UNP P39115
V	534	ALA	-	expression tag	UNP P39115
V	535	ALA	-	expression tag	UNP P39115
V	536	ALA	-	expression tag	UNP P39115
V	537	ALA	-	expression tag	UNP P39115
V	538	ALA	-	expression tag	UNP P39115
V	539	ALA	-	expression tag	UNP P39115
V	540	ALA	-	expression tag	UNP P39115
V	541	ALA	-	expression tag	UNP P39115
V	542	ALA	-	expression tag	UNP P39115

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	82	Total	C	N	O	0	0
			630	390	123	117		

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 26 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	63	Total	C	N	O	S	0	0
			499	312	91	91	5		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

- Molecule 32 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	212	Total	C	N	O	S	0	0
			1599	1015	273	306	5		

- Molecule 33 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1533	Total	C	N	O	P	0	0
			32891	14667	6034	10657	1533		

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	218	Total	C	N	O	S	0	0
			1757	1119	309	323	6		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	206	Total	C	N	O	S	0	0
			1619	1011	304	301	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	195	Total	C	N	O	S	0	0
			1568	991	291	284	2		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	164	Total	C	N	O	S	0	0
			1218	767	225	224	2		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	92	Total	C	N	O	S	0	0
			755	476	132	146	1		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	149	Total	C	N	O	S	0	0
			1181	740	220	215	6		

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	131	Total	C	N	O	S	0	0
			1036	655	191	187	3		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	125	Total	C	N	O	S	0	0
			966	599	191	175	1		

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	95	Total	C	N	O	S	0	0
			761	479	139	141	2		

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	114	Total	C	N	O	S	0	0
			838	516	164	156	2		

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	136	Total	C	N	O	S	0	0
			1052	653	211	186	2		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	m	108	Total	C	N	O		
			868	534	176	158	0	0

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	60	Total	C	N	O	S		
			497	317	98	77	5	0	0

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	85	Total	C	N	O	S		
			710	436	144	129	1	0	0

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	88	Total	C	N	O	S		
			695	441	128	124	2	0	0

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	84	Total	C	N	O	S		
			691	435	128	126	2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	64	Total	C	N	O	S		
			518	332	96	88	2	0	0

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	78	Total	C	N	O	S		
			633	409	112	110	2	0	0

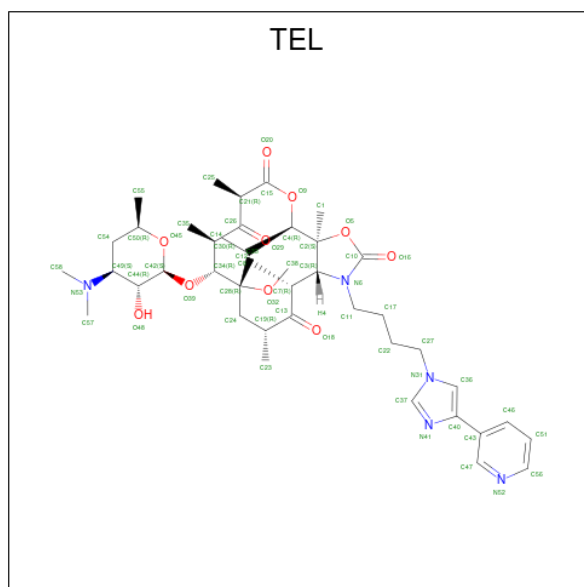
- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	83	Total	C	N	O	S	0	0
			637	390	130	116	1		

- Molecule 53 is a RNA chain called P-tRNA(Leu).

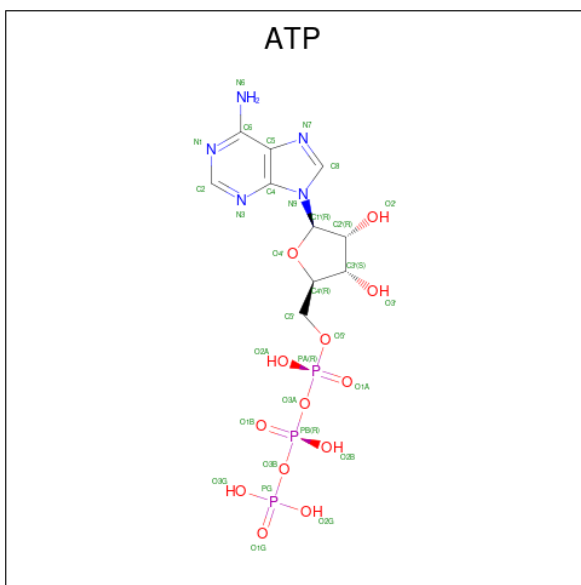
Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	75	Total	C	N	O	P	0	0
			1603	714	284	530	75		

- Molecule 54 is TELITHROMYCIN (CCD ID: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



Mol	Chain	Residues	Atoms				AltConf
54	A	1	Total	C	N	O	0
			58	43	5	10	

- Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

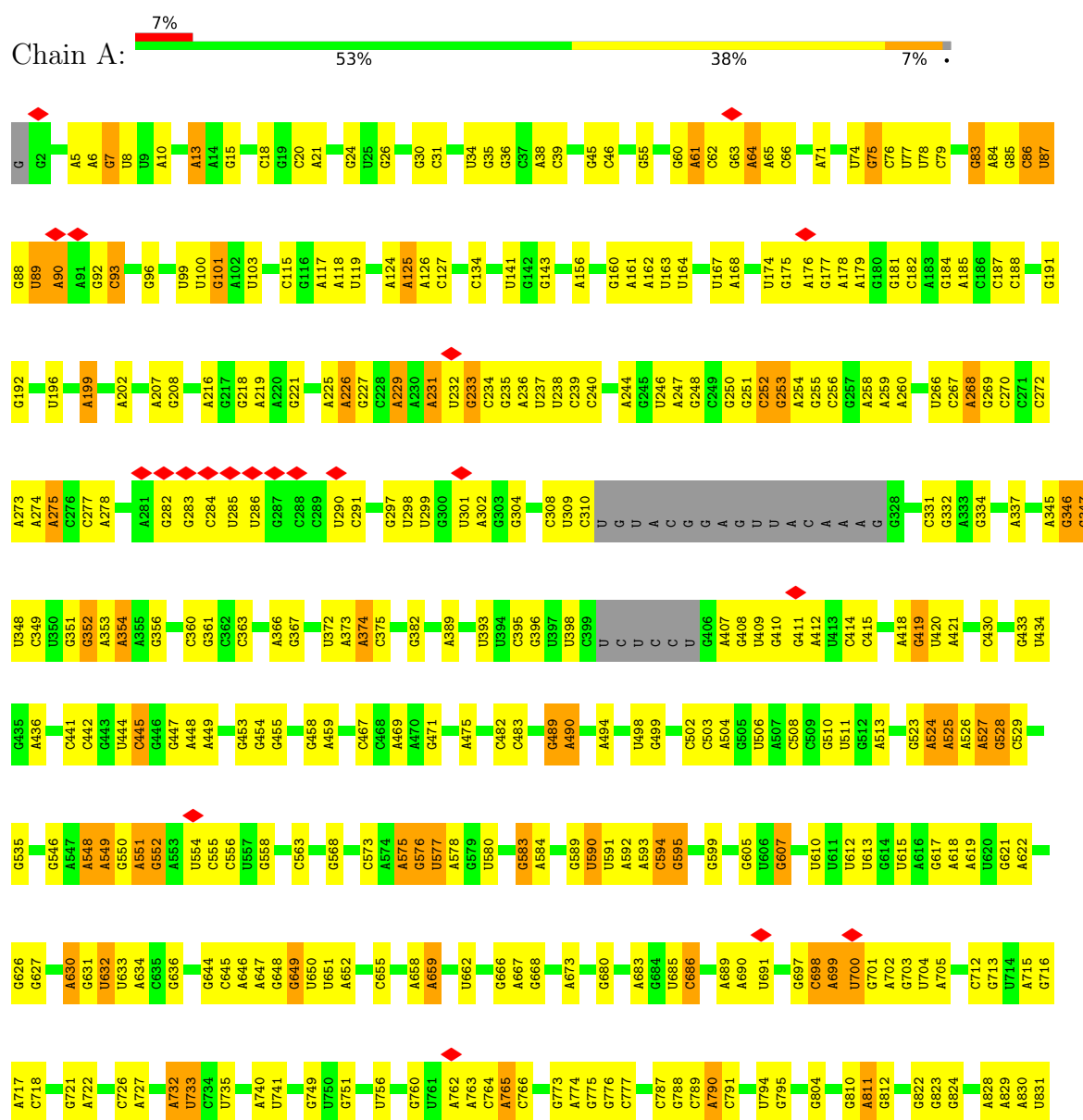


Mol	Chain	Residues	Atoms					AltConf
55	V	1	Total 31	C 10	N 5	O 13	P 3	0
55	V	1	Total 31	C 10	N 5	O 13	P 3	0

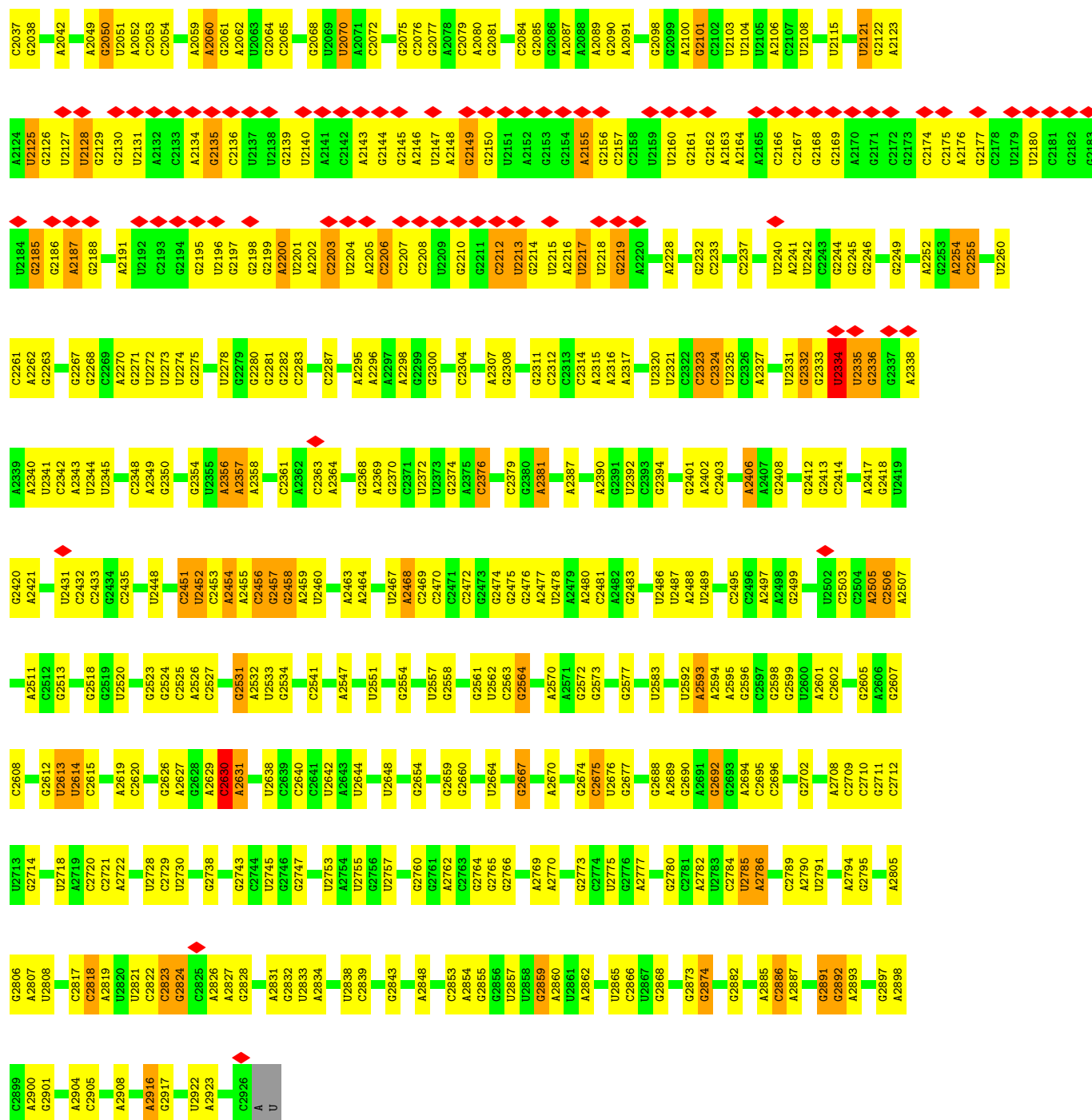
3 Residue-property plots

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

• Molecule 1: 23S rRNA

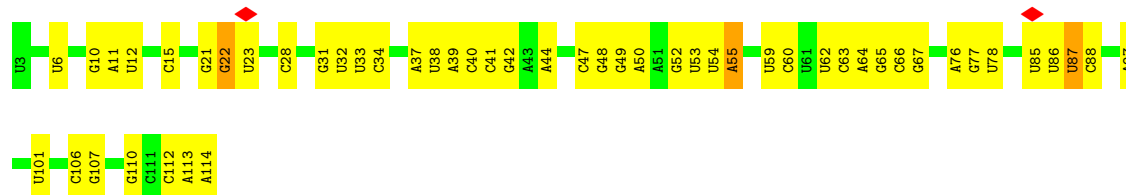




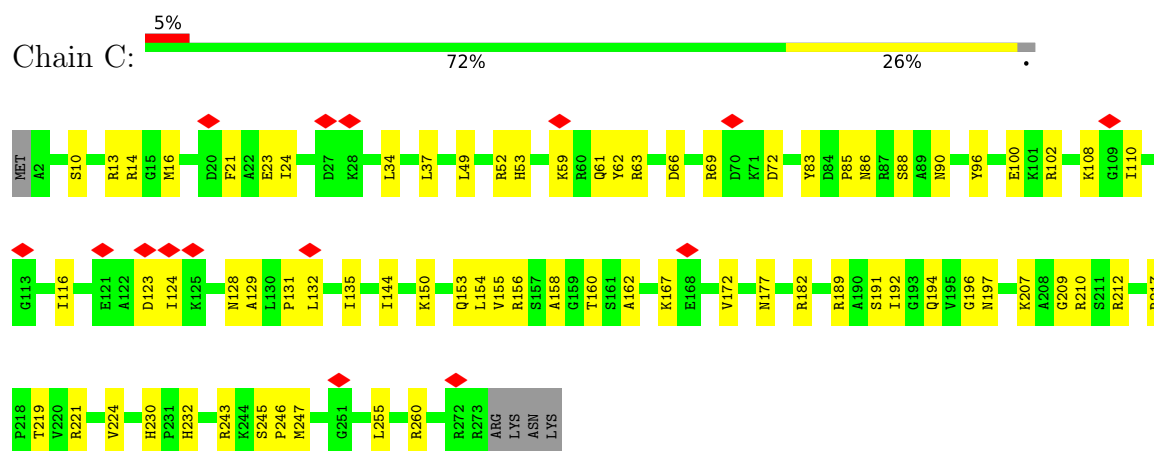


• Molecule 2: 5S rRNA

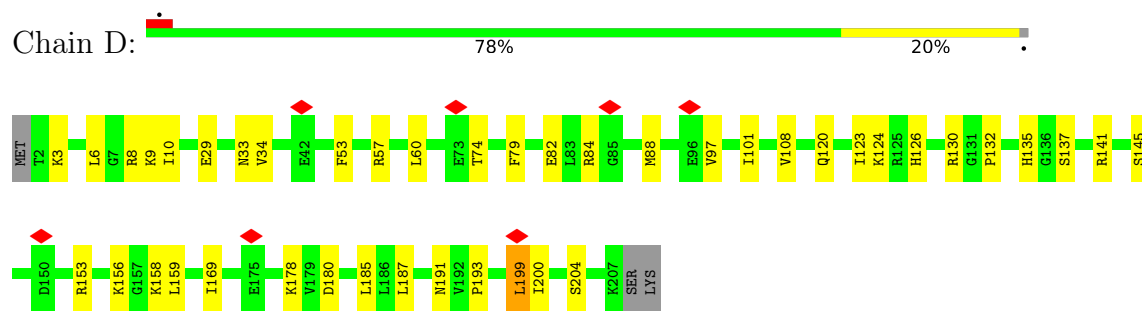
Chain B:



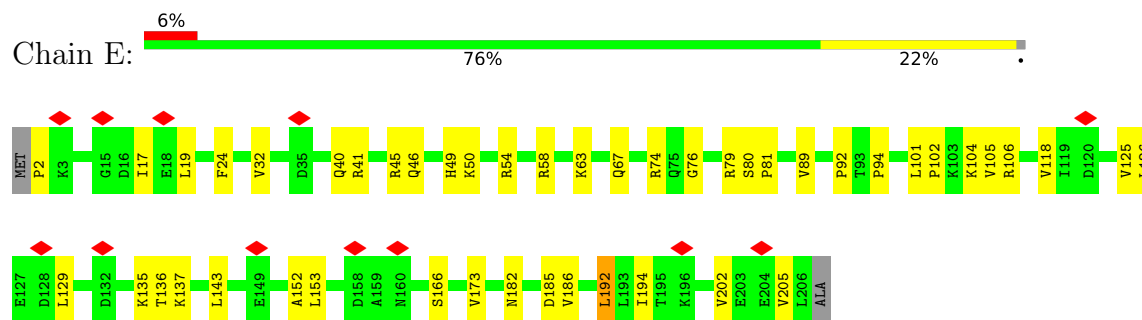
- Molecule 3: 50S ribosomal protein L2



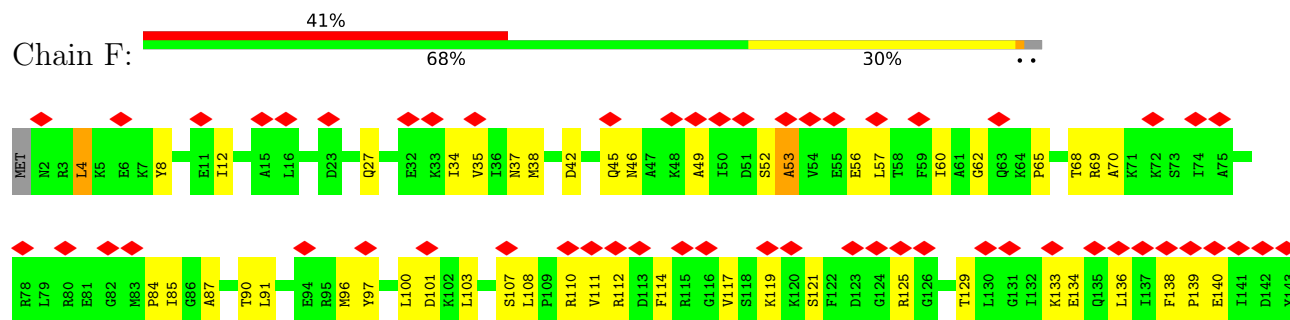
- Molecule 4: 50S ribosomal protein L3

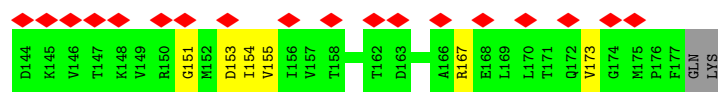


- Molecule 5: 50S ribosomal protein L4

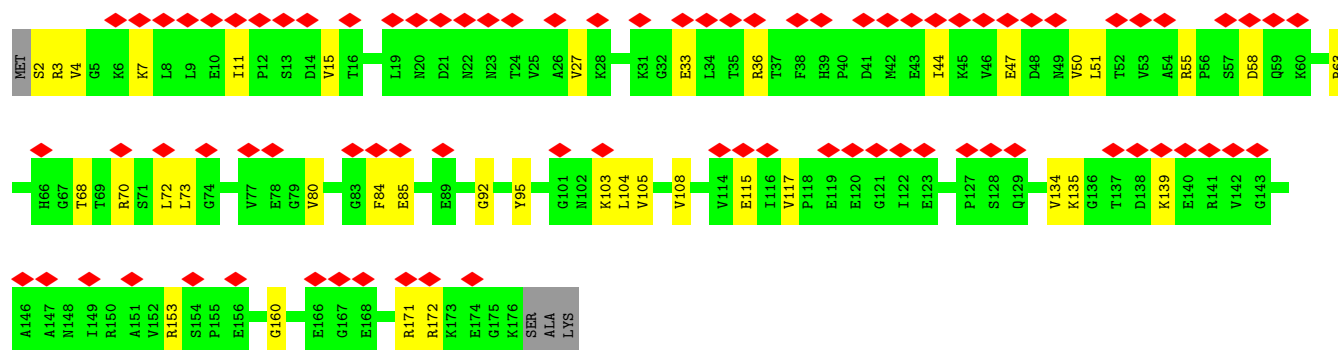
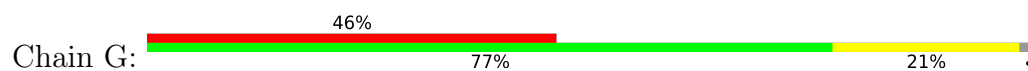


- Molecule 6: 50S ribosomal protein L5

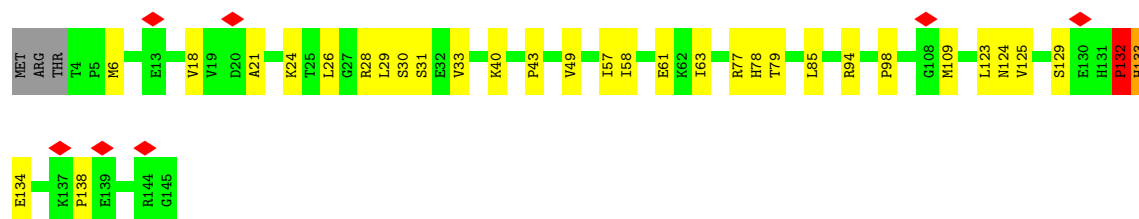
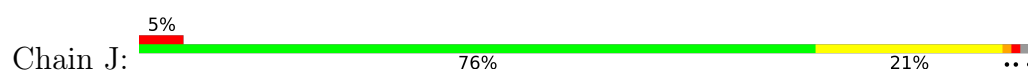




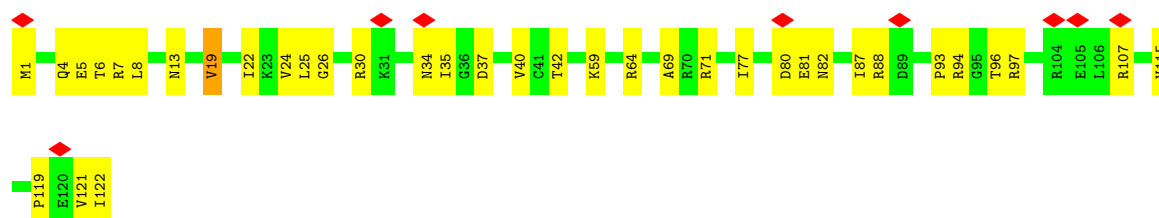
• Molecule 7: 50S ribosomal protein L6



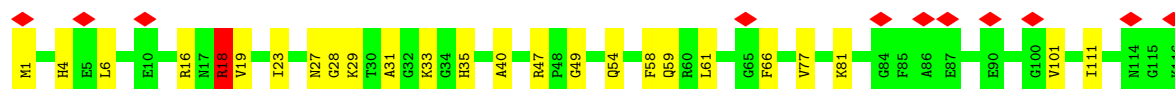
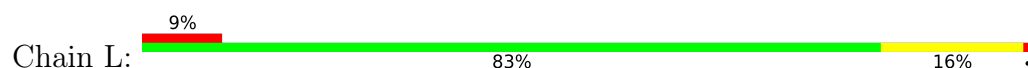
• Molecule 8: 50S ribosomal protein L13

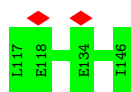


• Molecule 9: 50S ribosomal protein L14

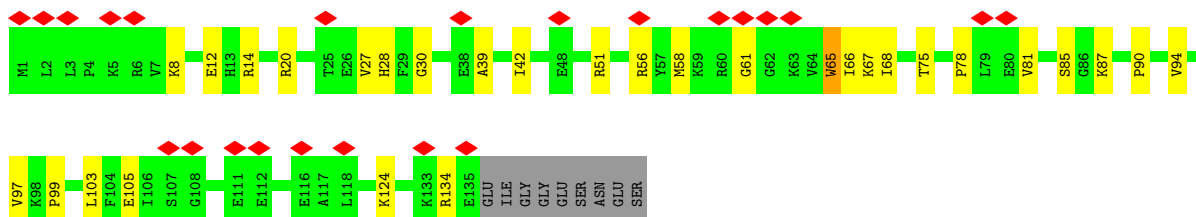
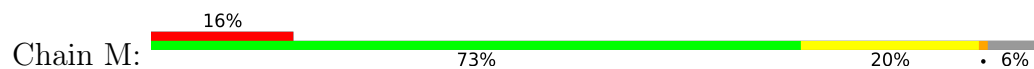


• Molecule 10: 50S ribosomal protein L15

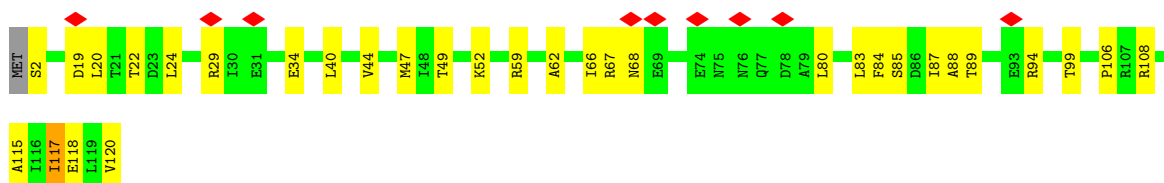




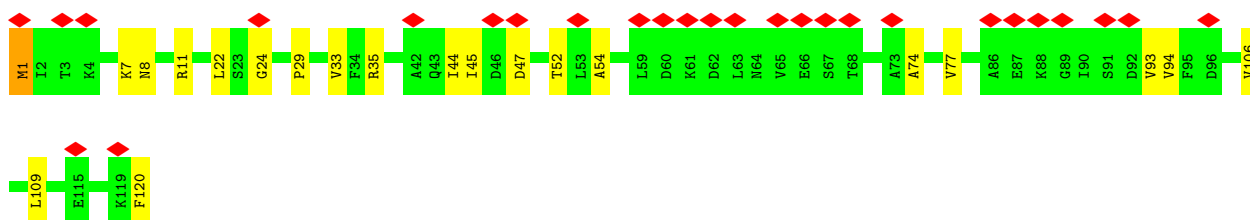
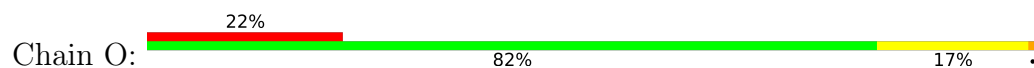
- Molecule 11: 50S ribosomal protein L16



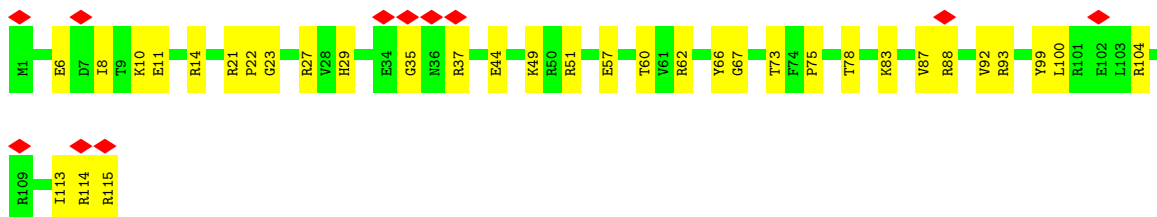
- Molecule 12: 50S ribosomal protein L17



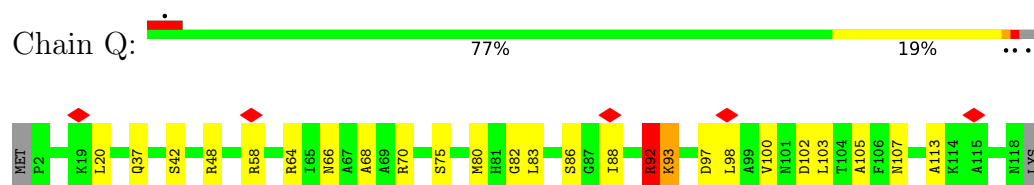
- Molecule 13: 50S ribosomal protein L18



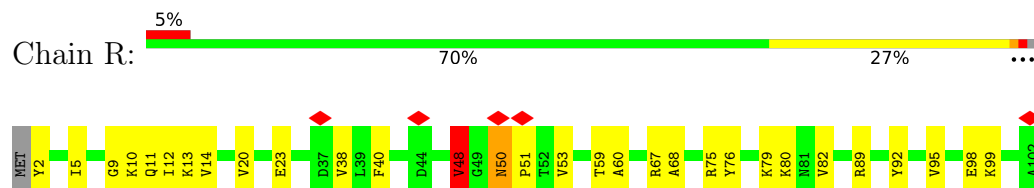
- Molecule 14: 50S ribosomal protein L19



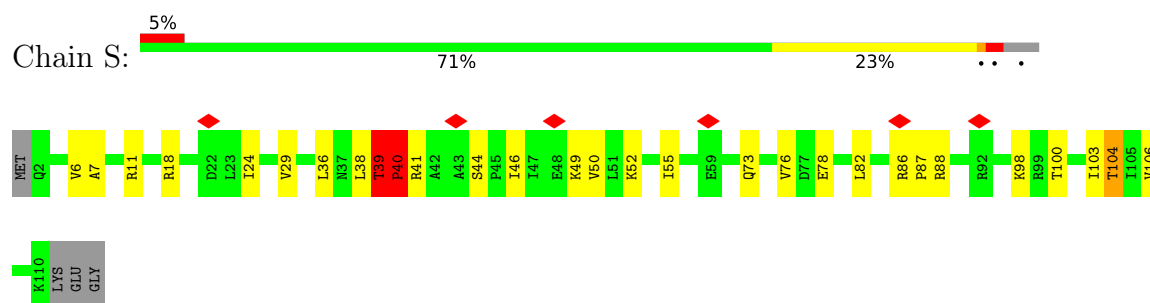
- Molecule 15: 50S ribosomal protein L20



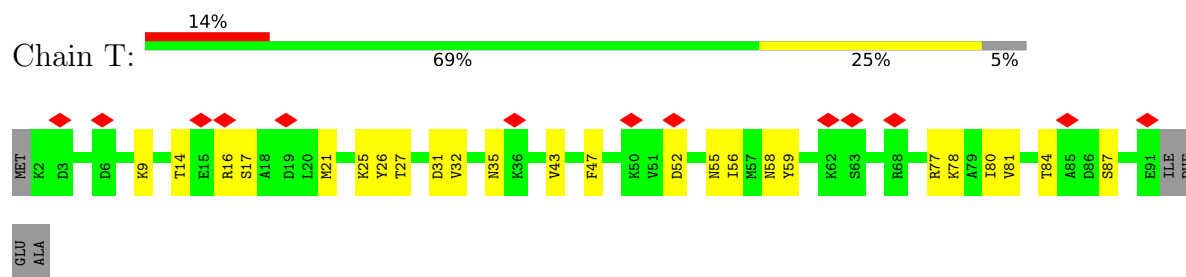
- Molecule 16: 50S ribosomal protein L21



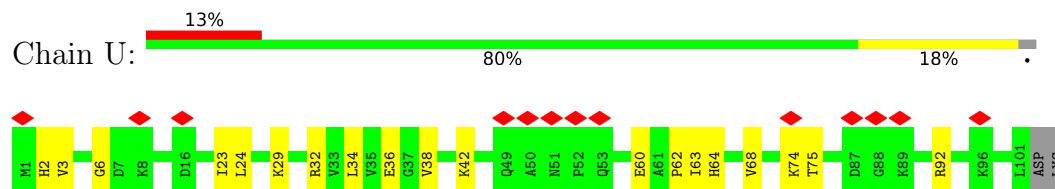
- Molecule 17: 50S ribosomal protein L22



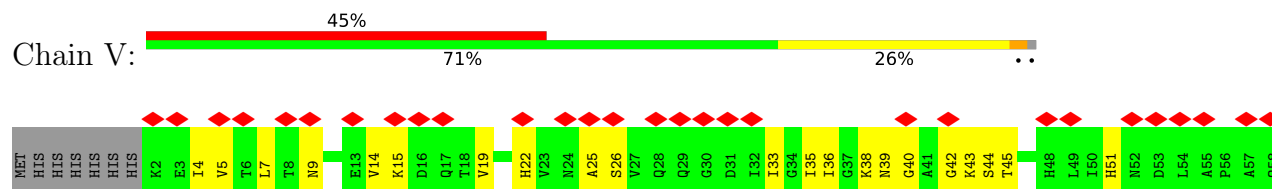
- Molecule 18: 50S ribosomal protein L23

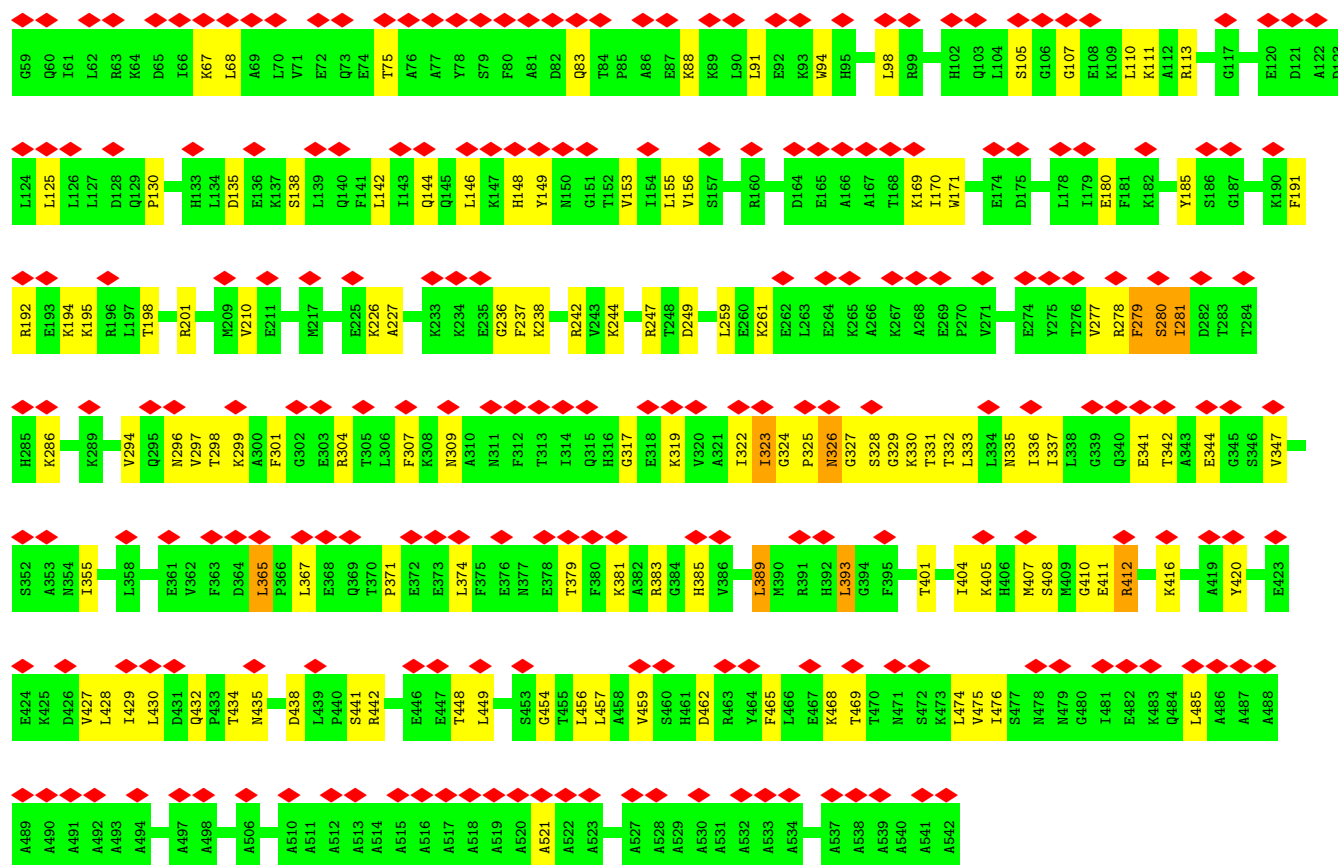


- Molecule 19: 50S ribosomal protein L24

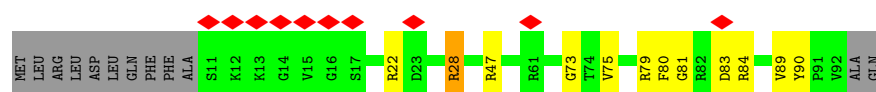
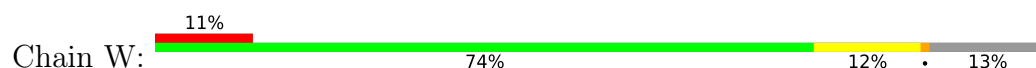


- Molecule 20: Nucleotide-binding protein ExpZ

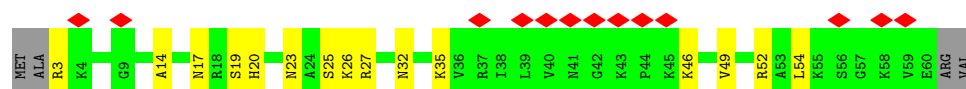




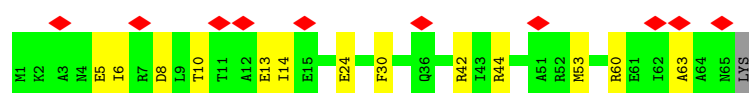
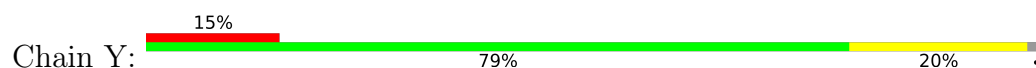
- Molecule 21: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L29



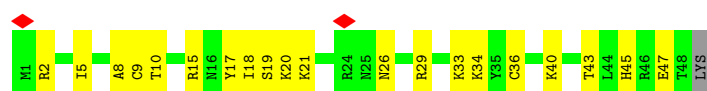
- Molecule 24: 50S ribosomal protein L30



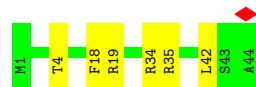
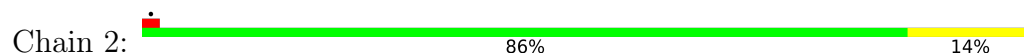
- Molecule 25: 50S ribosomal protein L32



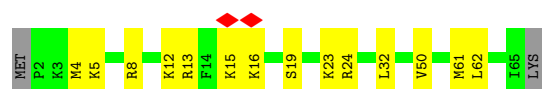
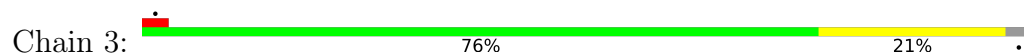
- Molecule 26: 50S ribosomal protein L33 1



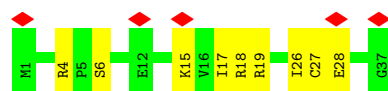
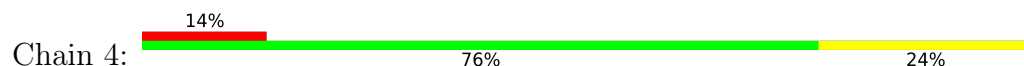
- Molecule 27: 50S ribosomal protein L34



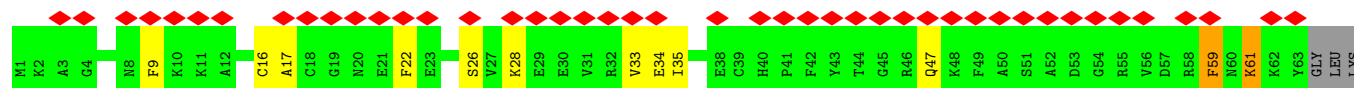
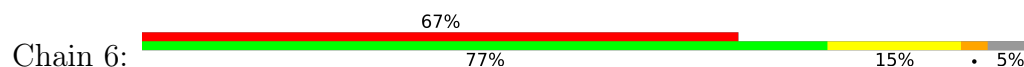
- Molecule 28: 50S ribosomal protein L35



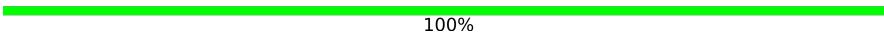
- Molecule 29: 50S ribosomal protein L36



- Molecule 30: 50S ribosomal protein L31

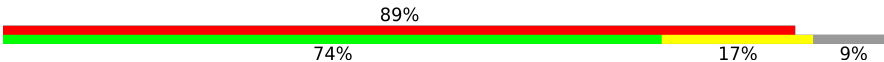


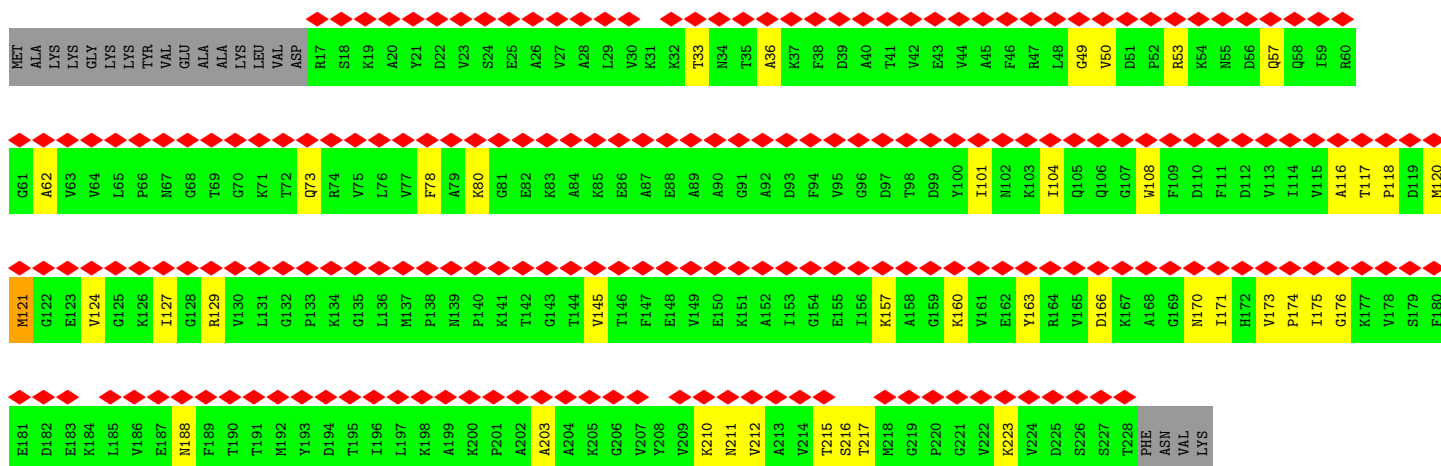
- Molecule 31: mRNA

Chain 7:  100%

There are no outlier residues recorded for this chain.

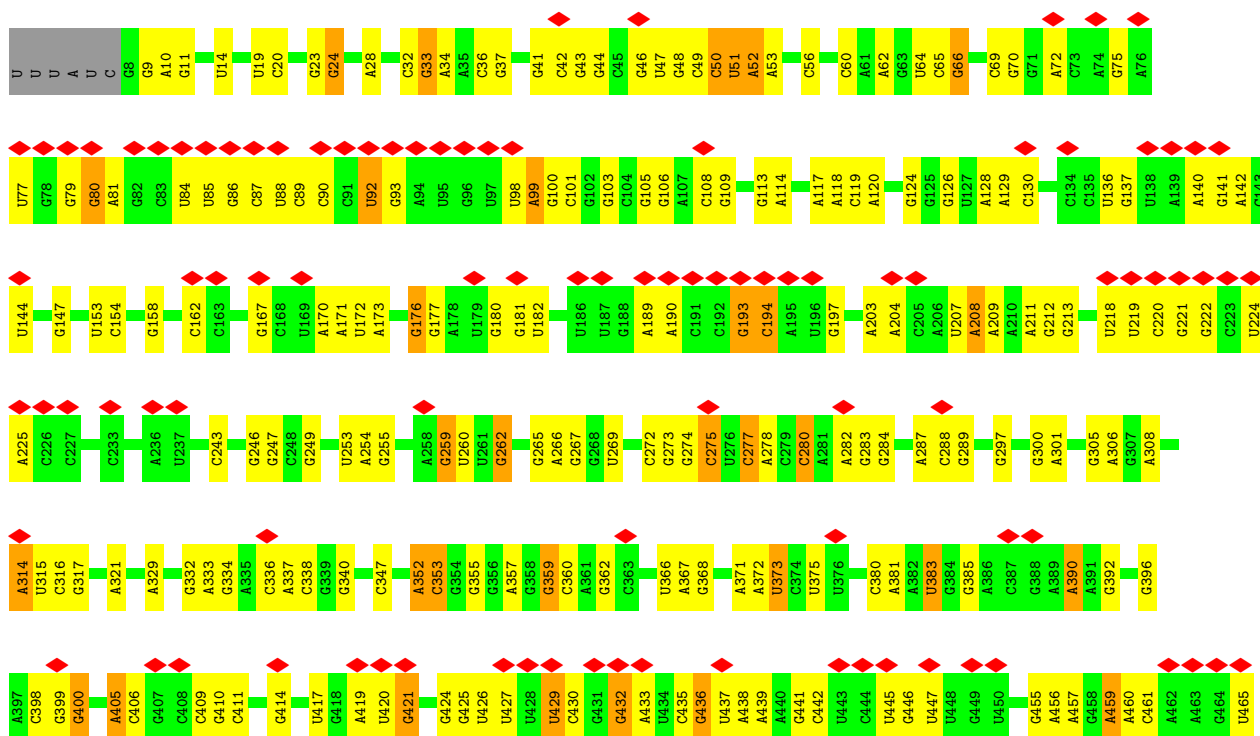
- Molecule 32: 50S ribosomal protein L1

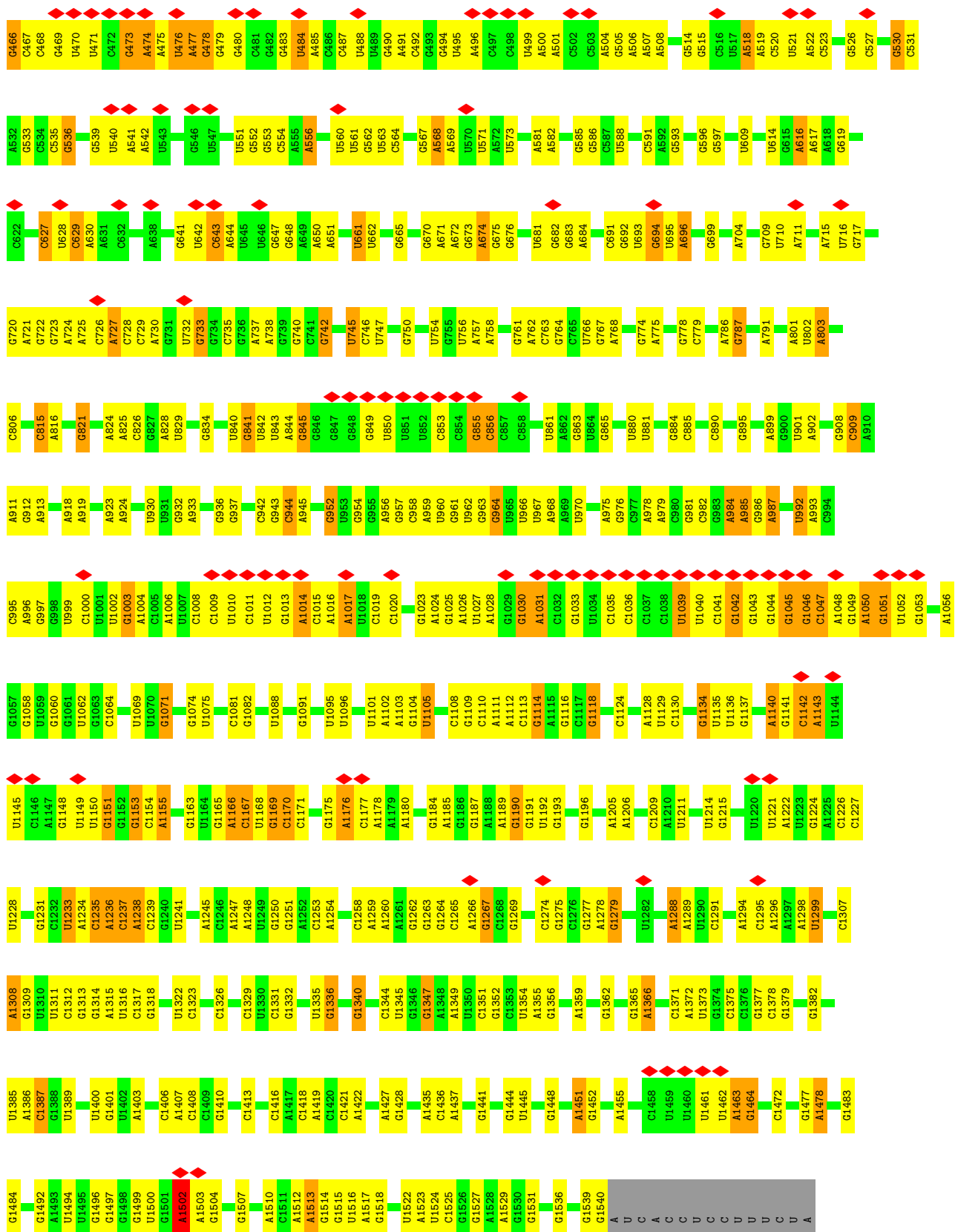
Chain 8:  89%

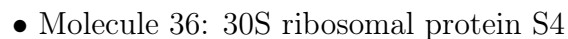
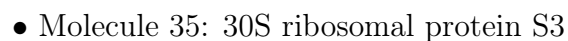


- Molecule 33: 16S rRNA

Chain a:  13%

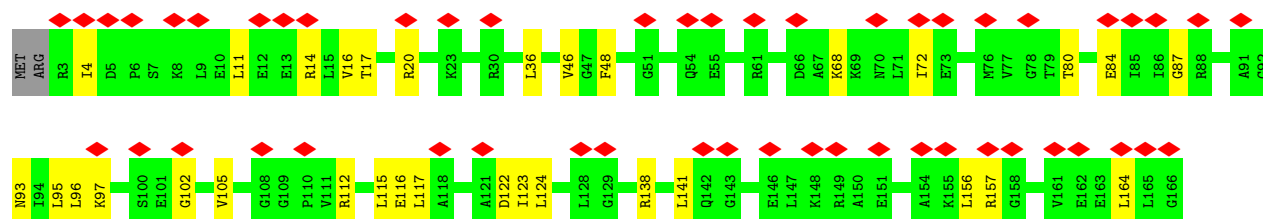
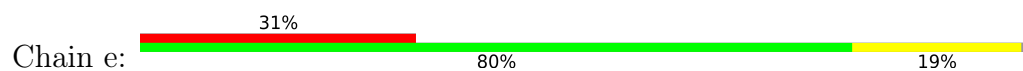




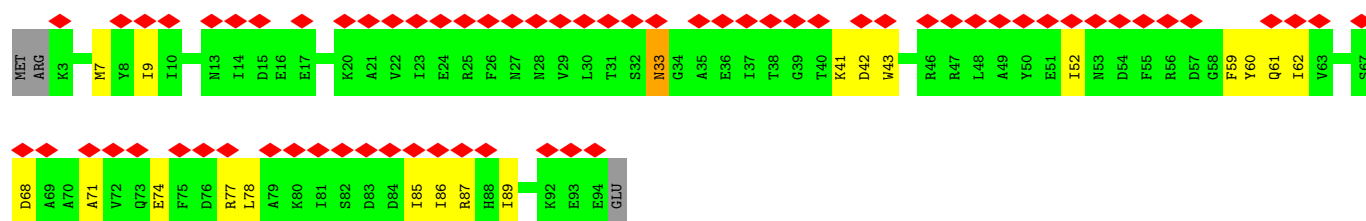
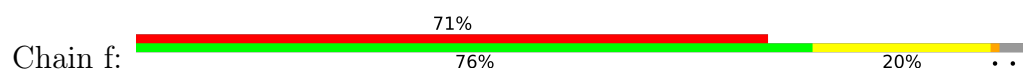




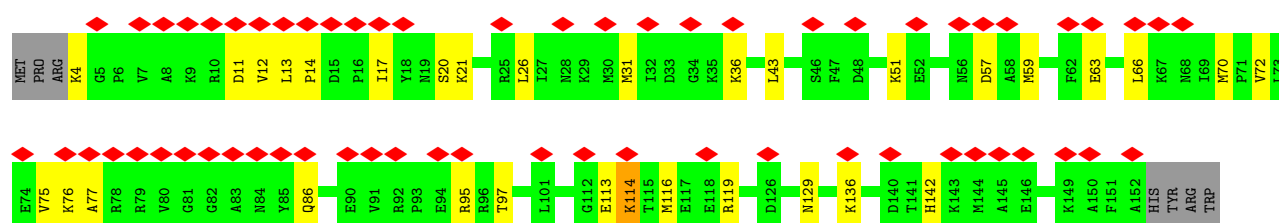
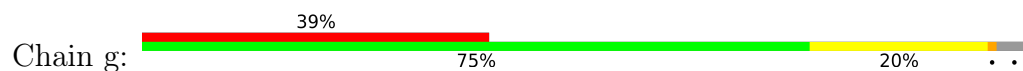
• Molecule 37: 30S ribosomal protein S5



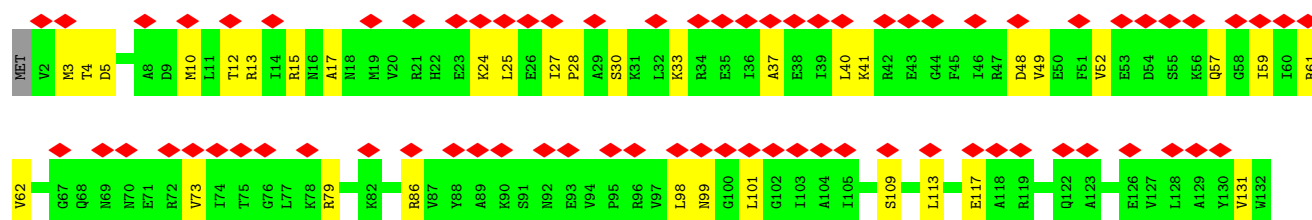
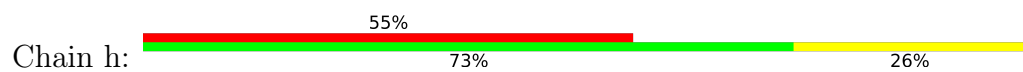
• Molecule 38: 30S ribosomal protein S6



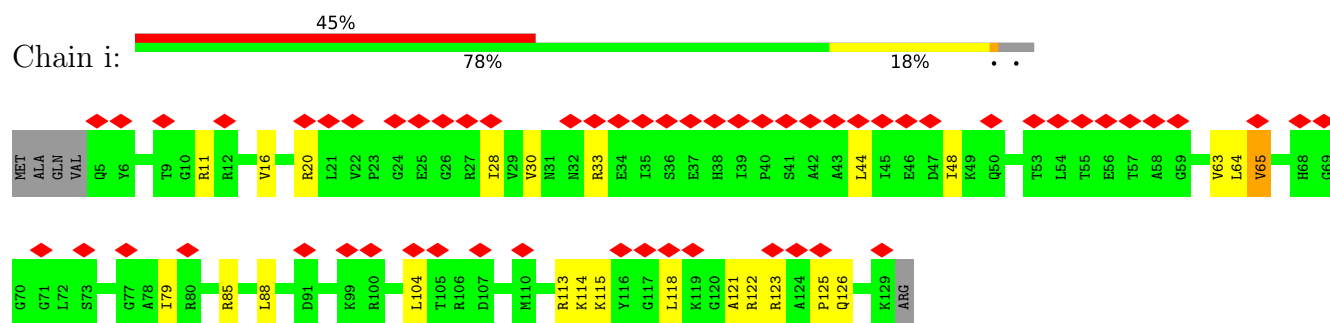
• Molecule 39: 30S ribosomal protein S7



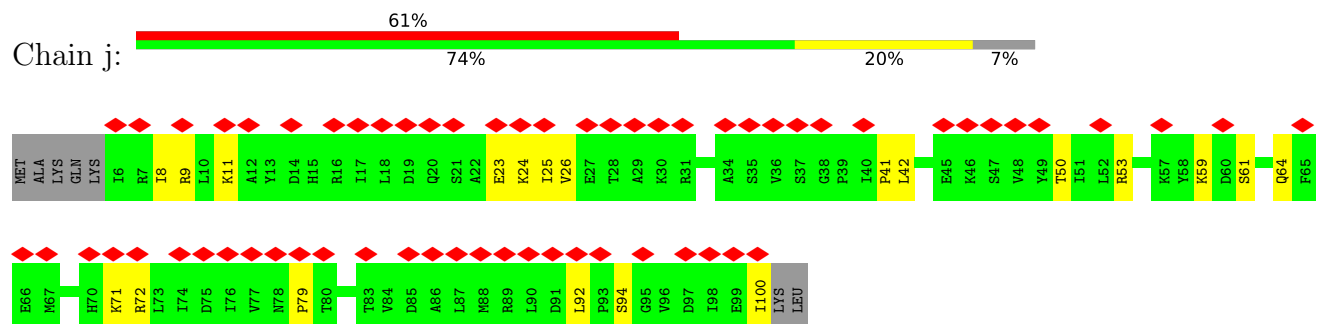
• Molecule 40: 30S ribosomal protein S8



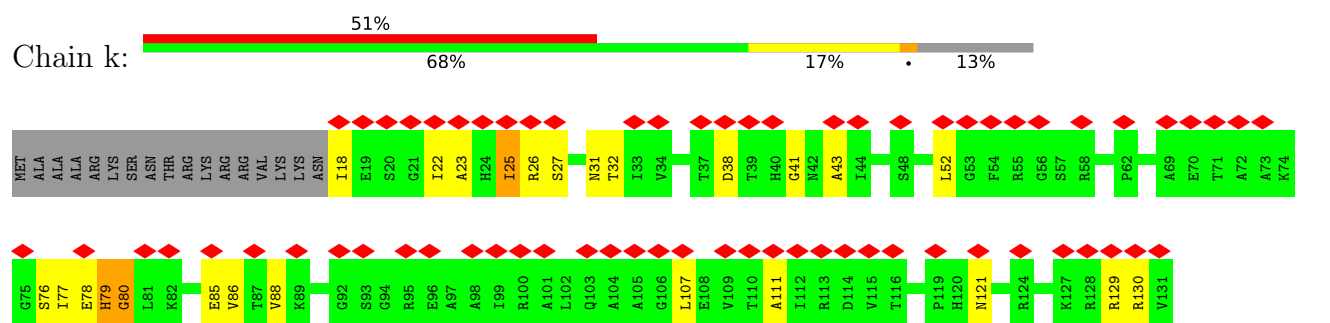
• Molecule 41: 30S ribosomal protein S9



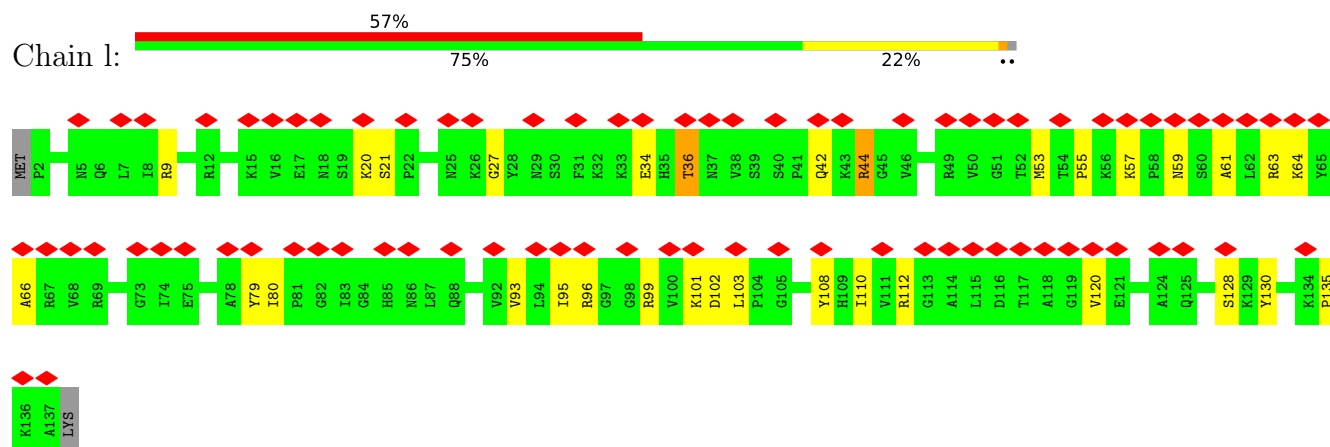
- Molecule 42: 30S ribosomal protein S10



- Molecule 43: 30S ribosomal protein S11

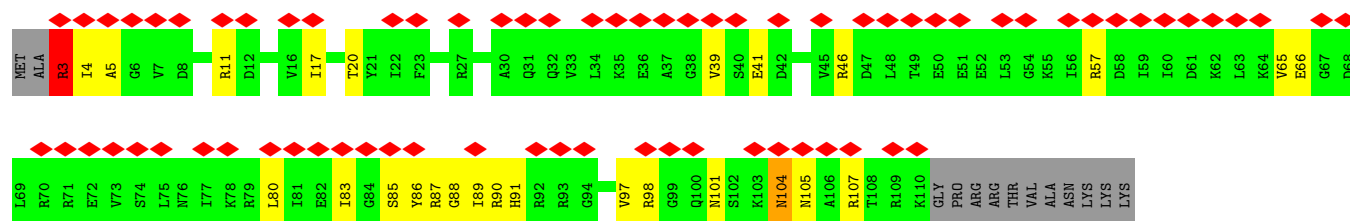


- Molecule 44: 30S ribosomal protein S12

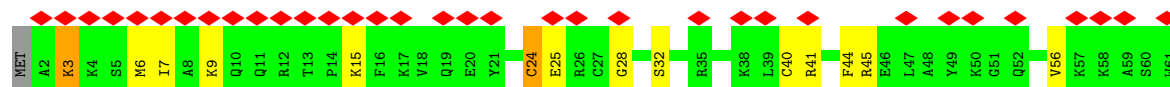
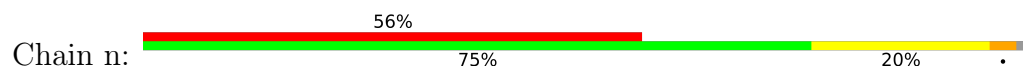


- Molecule 45: 30S ribosomal protein S13

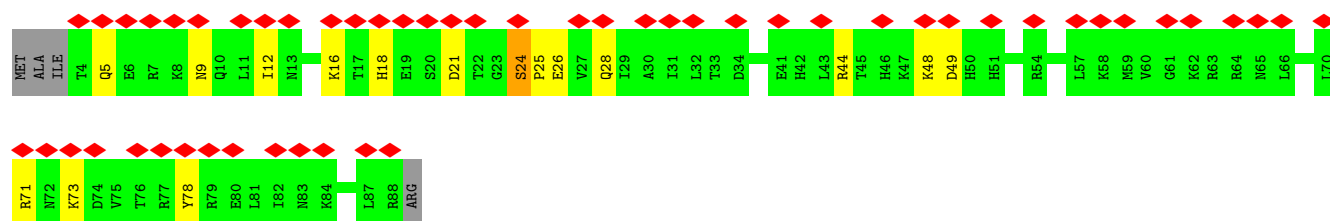
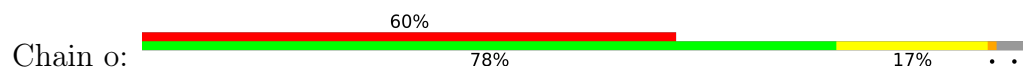




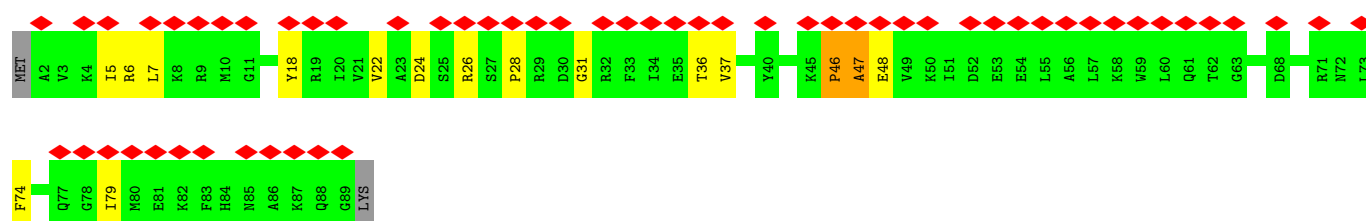
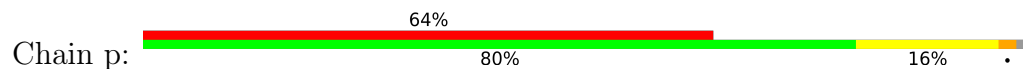
- Molecule 46: 30S ribosomal protein S14



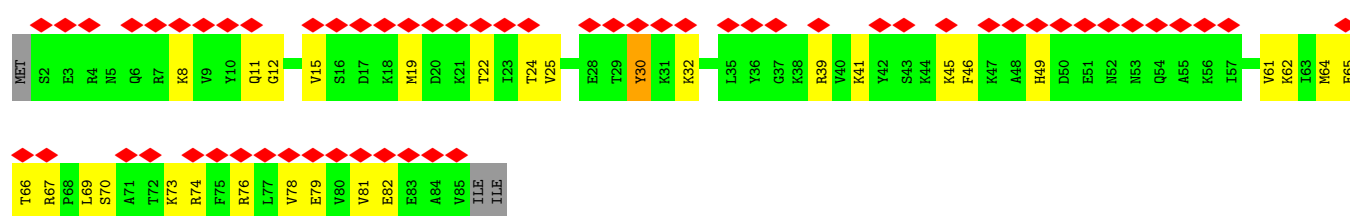
- Molecule 47: 30S ribosomal protein S15



- Molecule 48: 30S ribosomal protein S16



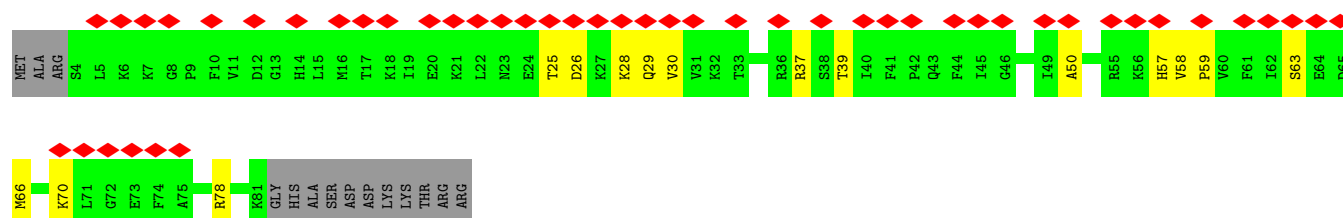
- Molecule 49: 30S ribosomal protein S17



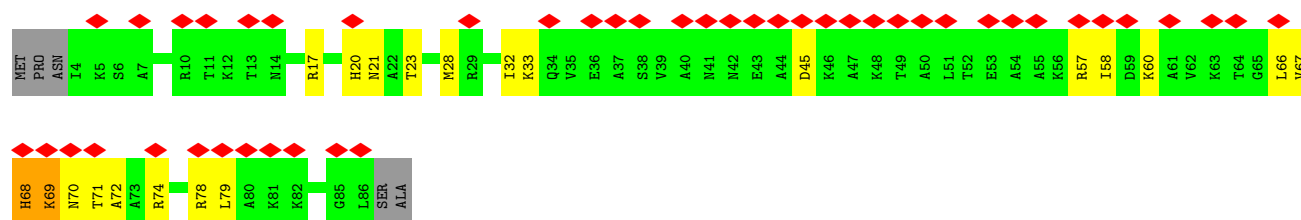
- Molecule 50: 30S ribosomal protein S18



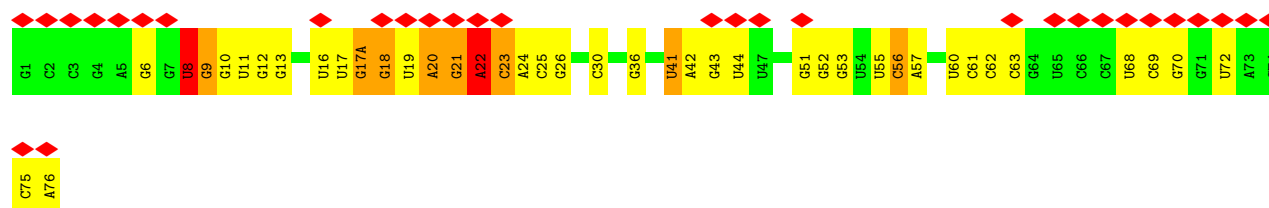
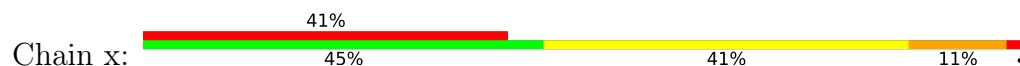
- Molecule 51: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S20



- Molecule 53: P-tRNA(Leu)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	28972	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 ($e^-/\text{\AA}^2$)	1.425	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.634	Depositor
Minimum map value	-0.379	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	381.96, 381.96, 381.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, TEL

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	0.52	2/69438 (0.0%)	0.61	7/108311 (0.0%)
2	B	0.40	0/2675	0.60	0/4170
3	C	0.60	0/2120	0.94	1/2845 (0.0%)
4	D	0.59	0/1591	0.89	0/2132
5	E	0.53	0/1580	0.81	0/2132
6	F	0.44	0/1405	0.93	1/1887 (0.1%)
7	G	0.37	0/1360	0.82	0/1832
8	J	0.57	0/1146	0.90	0/1542
9	K	0.57	0/927	0.92	0/1245
10	L	0.54	0/1093	0.94	1/1457 (0.1%)
11	M	0.52	0/1099	0.93	1/1468 (0.1%)
12	N	0.55	0/960	0.81	0/1284
13	O	0.43	0/921	0.87	0/1236
14	P	0.51	0/957	0.90	1/1279 (0.1%)
15	Q	0.63	1/952 (0.1%)	0.89	3/1266 (0.2%)
16	R	0.56	0/797	0.95	1/1070 (0.1%)
17	S	0.57	0/851	0.95	4/1146 (0.3%)
18	T	0.46	0/731	0.83	0/974
19	U	0.47	0/772	0.94	0/1032
20	V	0.39	0/4247	0.85	5/5736 (0.1%)
21	W	0.60	0/638	1.08	2/847 (0.2%)
22	X	0.44	0/448	0.91	0/596
23	Y	0.42	0/531	0.85	0/707
24	Z	0.46	0/457	0.92	0/613
25	0	0.56	0/433	0.93	0/574
26	1	0.50	0/406	0.93	0/540
27	2	0.60	0/370	0.84	0/483
28	3	0.56	0/519	0.82	0/680
29	4	0.46	0/299	0.79	0/393
30	6	0.38	0/509	0.98	2/678 (0.3%)
31	7	0.33	0/65	0.51	0/98
32	8	0.29	0/1624	0.78	1/2192 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.33	0/36826	0.57	7/57450 (0.0%)
34	b	0.32	0/1782	0.89	6/2392 (0.3%)
35	c	0.33	0/1641	0.82	0/2208
36	d	0.35	0/1598	0.93	4/2147 (0.2%)
37	e	0.38	0/1230	0.86	0/1655
38	f	0.28	0/766	0.75	0/1031
39	g	0.40	0/1196	0.89	3/1604 (0.2%)
40	h	0.36	0/1048	0.89	2/1407 (0.1%)
41	i	0.36	0/979	0.88	1/1315 (0.1%)
42	j	0.37	0/773	0.84	0/1044
43	k	0.37	0/852	1.02	5/1153 (0.4%)
44	l	0.36	0/1069	0.95	4/1435 (0.3%)
45	m	0.34	0/873	0.94	2/1166 (0.2%)
46	n	0.38	0/507	1.00	3/672 (0.4%)
47	o	0.31	0/718	0.72	0/960
48	p	0.37	0/708	0.93	4/950 (0.4%)
49	q	0.35	0/699	0.83	0/933
50	r	0.31	0/526	0.81	0/705
51	s	0.33	0/649	0.87	0/872
52	t	0.36	0/639	0.81	2/852 (0.2%)
53	x	0.36	0/1790	0.83	6/2787 (0.2%)
All	All	0.46	3/158790 (0.0%)	0.69	79/237183 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
4	D	0	1
6	F	0	3
8	J	0	1
10	L	0	2
13	O	0	1
15	Q	0	1
16	R	0	2
17	S	0	1
20	V	0	11
25	0	0	2
30	6	0	1
34	b	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	d	0	5
37	e	0	1
38	f	0	1
39	g	0	2
40	h	0	1
44	l	0	2
45	m	0	3
47	o	0	1
49	q	0	1
50	r	0	2
All	All	0	51

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	20	LEU	CA-C	-5.98	1.44	1.52
1	A	700	U	C1'-N1	5.90	1.57	1.48
1	A	1489	U	C1'-N1	5.67	1.55	1.47

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	k	80	GLY	N-CA-C	16.91	131.24	112.29
43	k	79	HIS	N-CA-C	-11.19	97.79	111.33
11	M	65	TRP	N-CA-C	8.59	121.76	111.02
33	a	1176	A	O5'-C5'-C4'	8.35	124.22	111.70
21	W	28	ARG	CB-CG-CD	7.66	128.93	111.30

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	153	GLN	Peptide
4	D	53	PHE	Peptide
6	F	117	VAL	Peptide
6	F	138	PHE	Peptide
6	F	53	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61997	0	31214	501	0
2	B	2392	0	1213	10	0
3	C	2083	0	2168	56	0
4	D	1569	0	1637	32	0
5	E	1561	0	1647	37	0
6	F	1386	0	1446	39	0
7	G	1342	0	1388	22	0
8	J	1123	0	1162	25	0
9	K	920	0	977	24	0
10	L	1081	0	1132	19	0
11	M	1076	0	1145	19	0
12	N	953	0	983	21	0
13	O	912	0	947	16	0
14	P	944	0	1020	26	0
15	Q	940	0	1005	21	0
16	R	786	0	826	19	0
17	S	842	0	899	18	0
18	T	725	0	770	18	0
19	U	762	0	821	11	0
20	V	4177	0	4221	202	0
21	W	630	0	644	9	0
22	X	444	0	487	11	0
23	Y	530	0	568	10	0
24	Z	455	0	491	14	0
25	0	426	0	441	12	0
26	1	401	0	413	16	0
27	2	367	0	410	5	0
28	3	512	0	564	13	0
29	4	296	0	342	8	0
30	6	499	0	491	10	0
31	7	60	0	32	0	0
32	8	1599	0	1640	48	0
33	a	32891	0	16559	347	0
34	b	1757	0	1830	29	0
35	c	1619	0	1658	31	0
36	d	1568	0	1604	33	0
37	e	1218	0	1300	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	f	755	0	746	14	0
39	g	1181	0	1235	23	0
40	h	1036	0	1095	20	0
41	i	966	0	1005	17	0
42	j	761	0	795	15	0
43	k	838	0	854	20	0
44	l	1052	0	1112	24	0
45	m	868	0	925	18	0
46	n	497	0	531	11	0
47	o	710	0	735	10	0
48	p	695	0	721	9	0
49	q	691	0	728	21	0
50	r	518	0	555	9	0
51	s	633	0	649	9	0
52	t	637	0	696	14	0
53	x	1603	0	808	17	0
54	A	58	0	65	16	0
55	V	62	0	24	59	0
All	All	146404	0	99374	1700	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1700 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:328:SER:HB3	20:V:476:ILE:CG2	1.25	1.64
20:V:43:LYS:CD	20:V:156:VAL:CG1	1.78	1.59
20:V:43:LYS:CE	20:V:156:VAL:HG11	1.39	1.49
20:V:328:SER:CB	20:V:476:ILE:CG2	1.92	1.44
20:V:43:LYS:NZ	20:V:156:VAL:HG11	1.28	1.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	270/277 (98%)	253 (94%)	17 (6%)	0	100	100
4	D	204/209 (98%)	195 (96%)	9 (4%)	0	100	100
5	E	203/207 (98%)	187 (92%)	16 (8%)	0	100	100
6	F	174/179 (97%)	159 (91%)	15 (9%)	0	100	100
7	G	173/179 (97%)	153 (88%)	20 (12%)	0	100	100
8	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	9	38
9	K	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
10	L	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
11	M	133/144 (92%)	125 (94%)	8 (6%)	0	100	100
12	N	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
13	O	118/120 (98%)	107 (91%)	11 (9%)	0	100	100
14	P	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
15	Q	115/119 (97%)	107 (93%)	6 (5%)	2 (2%)	7	35
16	R	99/102 (97%)	83 (84%)	15 (15%)	1 (1%)	12	44
17	S	107/113 (95%)	92 (86%)	13 (12%)	2 (2%)	6	33
18	T	88/95 (93%)	84 (96%)	4 (4%)	0	100	100
19	U	99/103 (96%)	86 (87%)	13 (13%)	0	100	100
20	V	539/548 (98%)	464 (86%)	73 (14%)	2 (0%)	30	62
21	W	80/94 (85%)	71 (89%)	9 (11%)	0	100	100
22	X	56/62 (90%)	46 (82%)	10 (18%)	0	100	100
23	Y	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
24	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
25	0	52/59 (88%)	49 (94%)	2 (4%)	1 (2%)	6	33
26	1	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
27	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
28	3	62/66 (94%)	60 (97%)	2 (3%)	0	100	100
29	4	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
30	6	61/66 (92%)	53 (87%)	8 (13%)	0	100	100
32	8	210/232 (90%)	192 (91%)	18 (9%)	0	100	100
34	b	216/246 (88%)	188 (87%)	24 (11%)	4 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	c	204/218 (94%)	185 (91%)	19 (9%)	0	100	100
36	d	193/200 (96%)	173 (90%)	18 (9%)	2 (1%)	12	44
37	e	162/166 (98%)	150 (93%)	12 (7%)	0	100	100
38	f	90/95 (95%)	83 (92%)	7 (8%)	0	100	100
39	g	147/156 (94%)	136 (92%)	11 (8%)	0	100	100
40	h	129/132 (98%)	107 (83%)	20 (16%)	2 (2%)	7	36
41	i	123/130 (95%)	104 (85%)	18 (15%)	1 (1%)	16	49
42	j	93/102 (91%)	83 (89%)	9 (10%)	1 (1%)	11	43
43	k	112/131 (86%)	100 (89%)	12 (11%)	0	100	100
44	l	134/138 (97%)	117 (87%)	16 (12%)	1 (1%)	18	51
45	m	106/121 (88%)	94 (89%)	11 (10%)	1 (1%)	14	47
46	n	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	7	35
47	o	83/89 (93%)	79 (95%)	3 (4%)	1 (1%)	10	41
48	p	86/90 (96%)	76 (88%)	7 (8%)	3 (4%)	3	23
49	q	82/87 (94%)	77 (94%)	5 (6%)	0	100	100
50	r	62/79 (78%)	57 (92%)	5 (8%)	0	100	100
51	s	76/92 (83%)	66 (87%)	10 (13%)	0	100	100
52	t	81/88 (92%)	76 (94%)	3 (4%)	2 (2%)	4	28
All	All	5956/6298 (95%)	5382 (90%)	545 (9%)	29 (0%)	26	57

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	J	133	HIS
15	Q	93	LYS
17	S	40	PRO
20	V	280	SER
34	b	18	HIS

5.3.2 Protein sidechains ⓘ

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	220/225 (98%)	220 (100%)	0	100	100
4	D	167/170 (98%)	165 (99%)	2 (1%)	63	73
5	E	169/170 (99%)	167 (99%)	2 (1%)	63	73
6	F	151/154 (98%)	149 (99%)	2 (1%)	61	72
7	G	148/151 (98%)	147 (99%)	1 (1%)	76	78
8	J	120/123 (98%)	117 (98%)	3 (2%)	42	63
9	K	101/101 (100%)	100 (99%)	1 (1%)	68	75
10	L	110/110 (100%)	109 (99%)	1 (1%)	70	76
11	M	109/116 (94%)	107 (98%)	2 (2%)	51	69
12	N	99/100 (99%)	98 (99%)	1 (1%)	68	75
13	O	93/93 (100%)	93 (100%)	0	100	100
14	P	100/100 (100%)	100 (100%)	0	100	100
15	Q	96/98 (98%)	96 (100%)	0	100	100
16	R	83/84 (99%)	82 (99%)	1 (1%)	63	73
17	S	90/93 (97%)	87 (97%)	3 (3%)	33	58
18	T	81/85 (95%)	81 (100%)	0	100	100
19	U	85/87 (98%)	85 (100%)	0	100	100
20	V	424/431 (98%)	419 (99%)	5 (1%)	63	73
21	W	64/74 (86%)	64 (100%)	0	100	100
22	X	47/50 (94%)	47 (100%)	0	100	100
23	Y	56/57 (98%)	56 (100%)	0	100	100
24	Z	52/53 (98%)	52 (100%)	0	100	100
25	0	48/53 (91%)	46 (96%)	2 (4%)	26	52
26	1	46/47 (98%)	46 (100%)	0	100	100
27	2	39/39 (100%)	39 (100%)	0	100	100
28	3	54/56 (96%)	52 (96%)	2 (4%)	30	56
29	4	35/35 (100%)	35 (100%)	0	100	100
30	6	53/55 (96%)	53 (100%)	0	100	100
32	8	169/185 (91%)	168 (99%)	1 (1%)	78	79
34	b	189/212 (89%)	187 (99%)	2 (1%)	65	74
35	c	168/178 (94%)	167 (99%)	1 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	d	169/173 (98%)	165 (98%)	4 (2%)	43	64
37	e	128/130 (98%)	125 (98%)	3 (2%)	44	64
38	f	81/84 (96%)	80 (99%)	1 (1%)	63	73
39	g	125/132 (95%)	125 (100%)	0	100	100
40	h	111/112 (99%)	111 (100%)	0	100	100
41	i	98/102 (96%)	97 (99%)	1 (1%)	68	75
42	j	86/92 (94%)	85 (99%)	1 (1%)	63	73
43	k	86/100 (86%)	84 (98%)	2 (2%)	44	64
44	l	114/116 (98%)	114 (100%)	0	100	100
45	m	94/104 (90%)	94 (100%)	0	100	100
46	n	53/54 (98%)	53 (100%)	0	100	100
47	o	80/83 (96%)	80 (100%)	0	100	100
48	p	74/76 (97%)	74 (100%)	0	100	100
49	q	77/80 (96%)	77 (100%)	0	100	100
50	r	56/64 (88%)	56 (100%)	0	100	100
51	s	70/81 (86%)	70 (100%)	0	100	100
52	t	66/70 (94%)	66 (100%)	0	100	100
All	All	5034/5238 (96%)	4990 (99%)	44 (1%)	68	76

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	8	121	MET
36	d	172	LEU
34	b	179	LEU
36	d	22	THR
37	e	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
29	4	36	GLN
36	d	85	ASN
50	r	25	HIS
32	8	67	ASN

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Mol	Chain	Res	Type
34	b	93	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2879/2928 (98%)	864 (30%)	90 (3%)
2	B	111/112 (99%)	40 (36%)	3 (2%)
31	7	2/3 (66%)	0	0
33	a	1532/1554 (98%)	412 (26%)	0
53	x	73/75 (97%)	29 (39%)	0
All	All	4597/4672 (98%)	1345 (29%)	93 (2%)

5 of 1345 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	U
1	A	10	A
1	A	13	A
1	A	18	C

5 of 93 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1530	G
1	A	1883	A
1	A	1543	U
1	A	1751	U
1	A	2127	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	TEL	A	3001	-	60,62,62	1.34	5 (8%)	78,92,92	1.98	17 (21%)
55	ATP	V	900	-	32,33,33	1.29	5 (15%)	48,52,52	1.89	11 (22%)
55	ATP	V	901	-	32,33,33	1.38	6 (18%)	48,52,52	1.80	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	TEL	A	3001	-	1/1/19/19	16/73/108/108	0/4/5/5
55	ATP	V	900	-	-	3/22/38/38	0/3/3/3
55	ATP	V	901	-	-	5/22/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A	3001	TEL	O5-C10	5.76	1.45	1.35
54	A	3001	TEL	O9-C15	5.01	1.45	1.34
55	V	901	ATP	C5-C4	4.57	1.47	1.39
55	V	900	ATP	C5-C4	4.19	1.46	1.39
54	A	3001	TEL	C40-N41	-3.21	1.35	1.38

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A	3001	TEL	O9-C15-C21	9.49	120.30	110.93
55	V	900	ATP	C5-C4-N3	-5.98	118.48	126.72
54	A	3001	TEL	C17-C11-N6	-5.49	104.94	113.25
55	V	901	ATP	C5-C4-N3	-5.30	119.42	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	V	900	ATP	N3-C4-N9	4.80	135.34	127.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
54	A	3001	TEL	C21

5 of 24 torsion outliers are listed below:

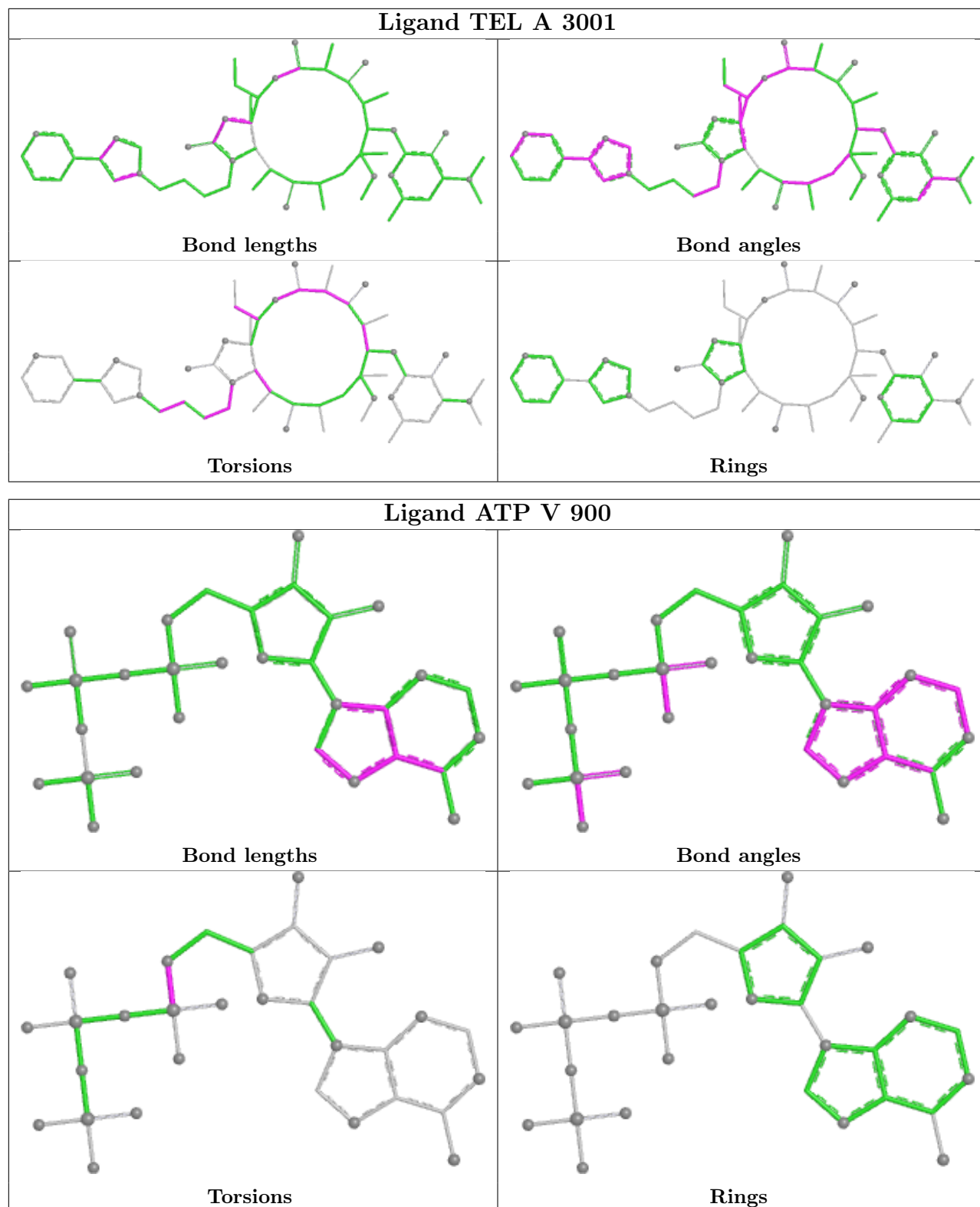
Mol	Chain	Res	Type	Atoms
54	A	3001	TEL	C15-C21-C26-O29
54	A	3001	TEL	C15-C21-C26-C30
55	V	900	ATP	C5'-O5'-PA-O1A
55	V	900	ATP	C5'-O5'-PA-O3A
55	V	901	ATP	C5'-O5'-PA-O1A

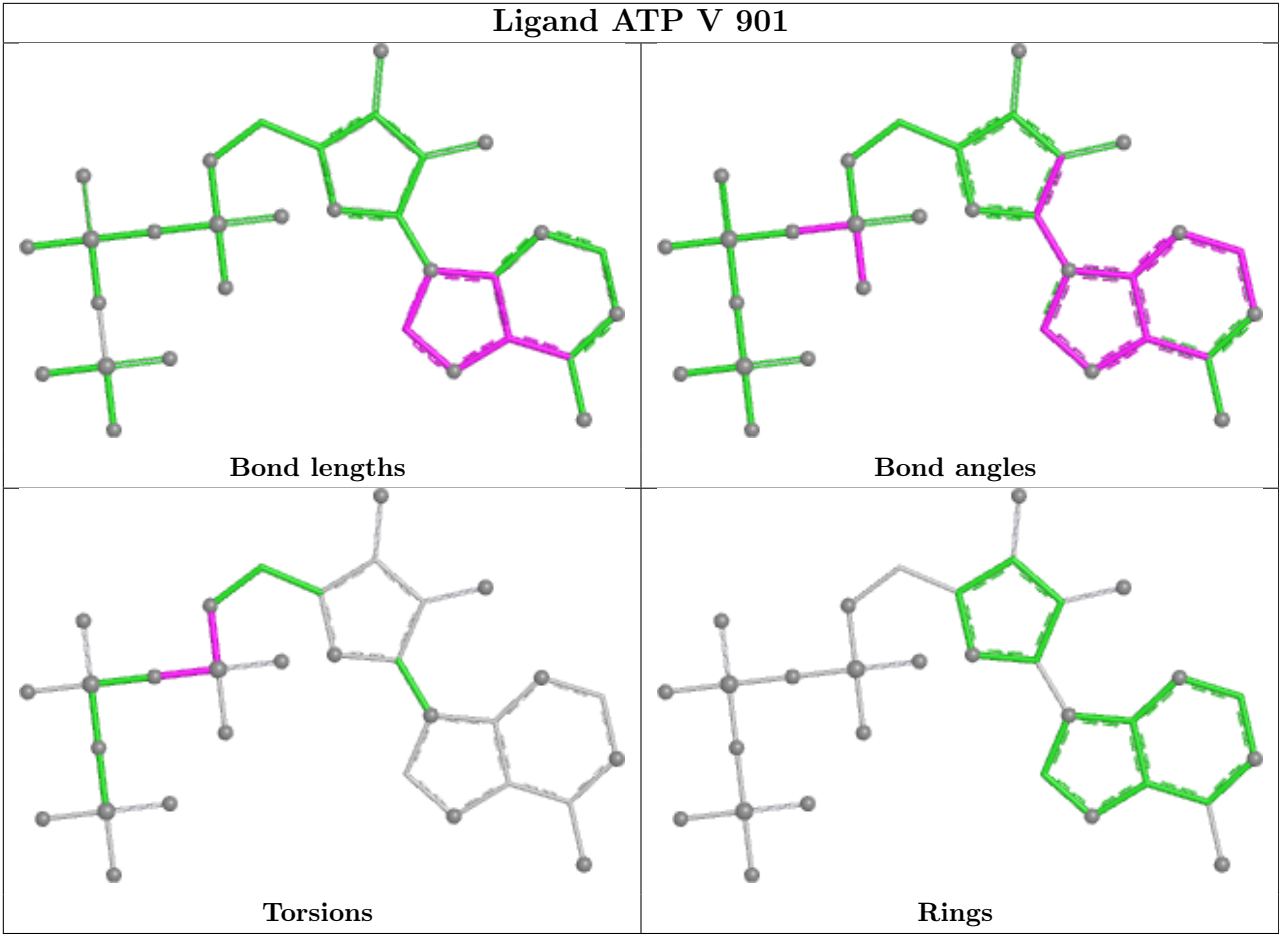
There are no ring outliers.

3 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	A	3001	TEL	16	0
55	V	900	ATP	24	0
55	V	901	ATP	35	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
53	x	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	44:U	O3'	47:U	P	14.81
1	A	182:C	O3'	183:A	P	6.43
1	A	1449:C	O3'	1450:C	P	4.34
1	A	1451:U	O3'	1452:C	P	3.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1452:C	O3'	1453:A	P	3.25

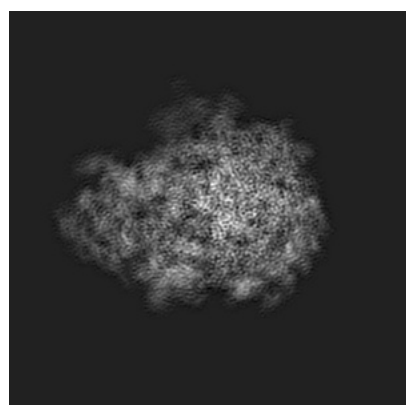
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0177. These allow visual inspection of the internal detail of the map and identification of artifacts.

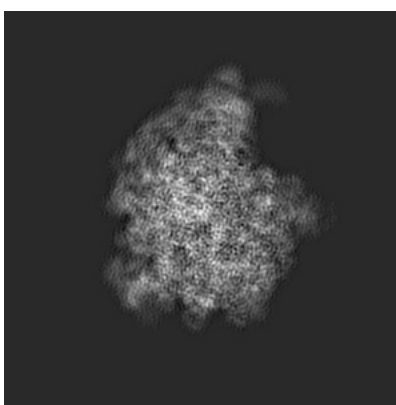
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

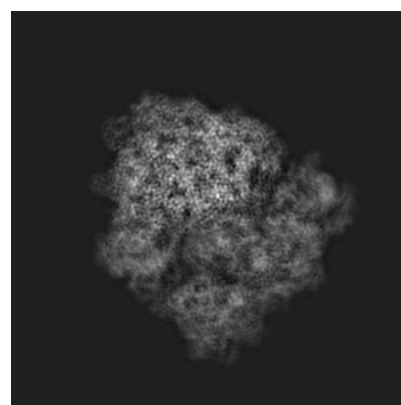
6.1.1 Primary map



X



Y

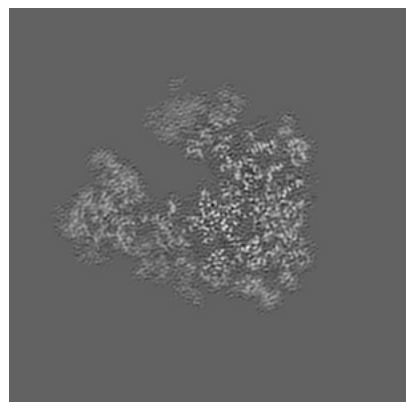


Z

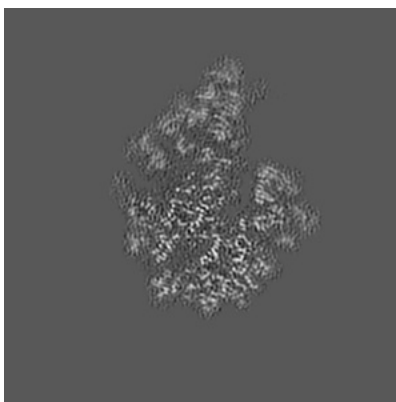
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

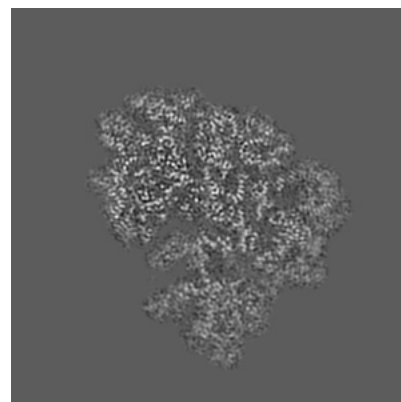
6.2.1 Primary map



X Index: 180



Y Index: 180

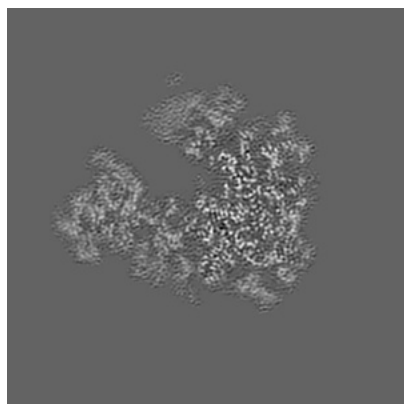


Z Index: 180

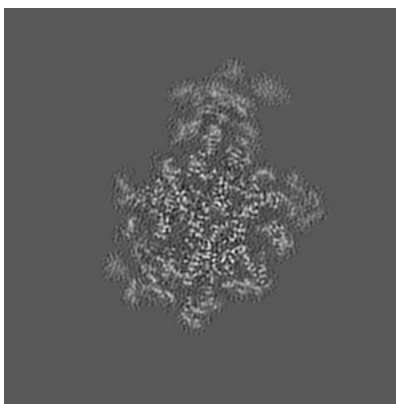
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

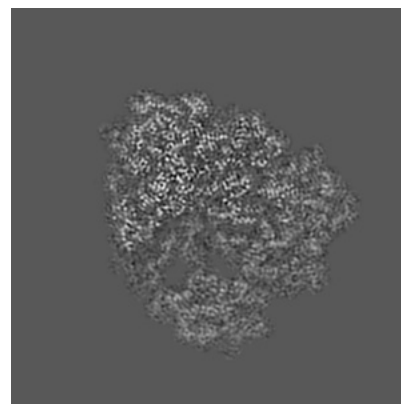
6.3.1 Primary map



X Index: 177



Y Index: 199

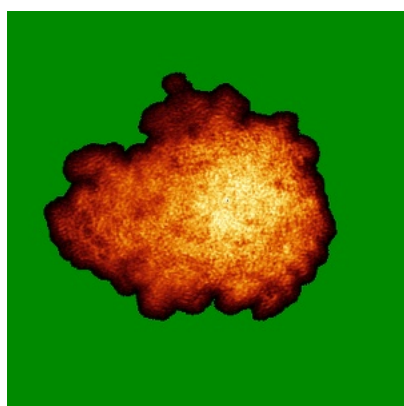


Z Index: 189

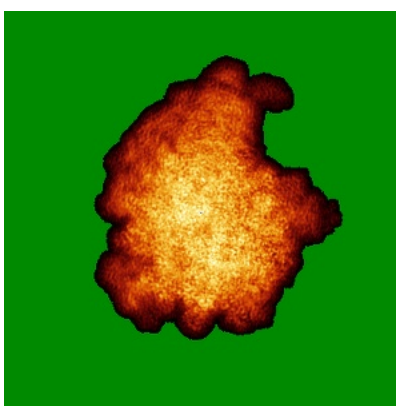
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

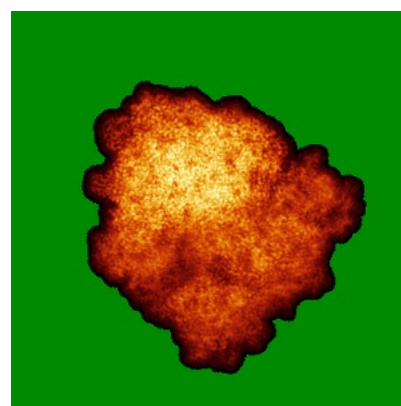
6.4.1 Primary map



X



Y

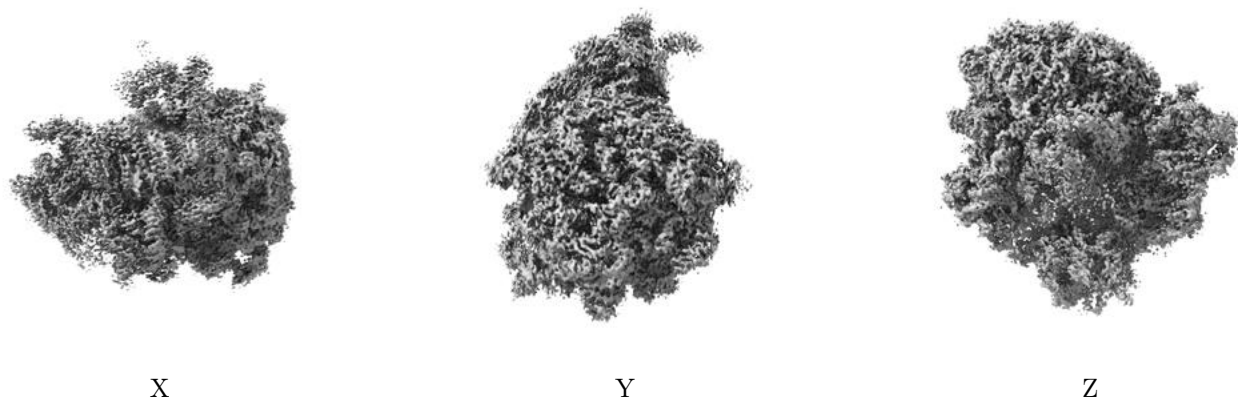


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

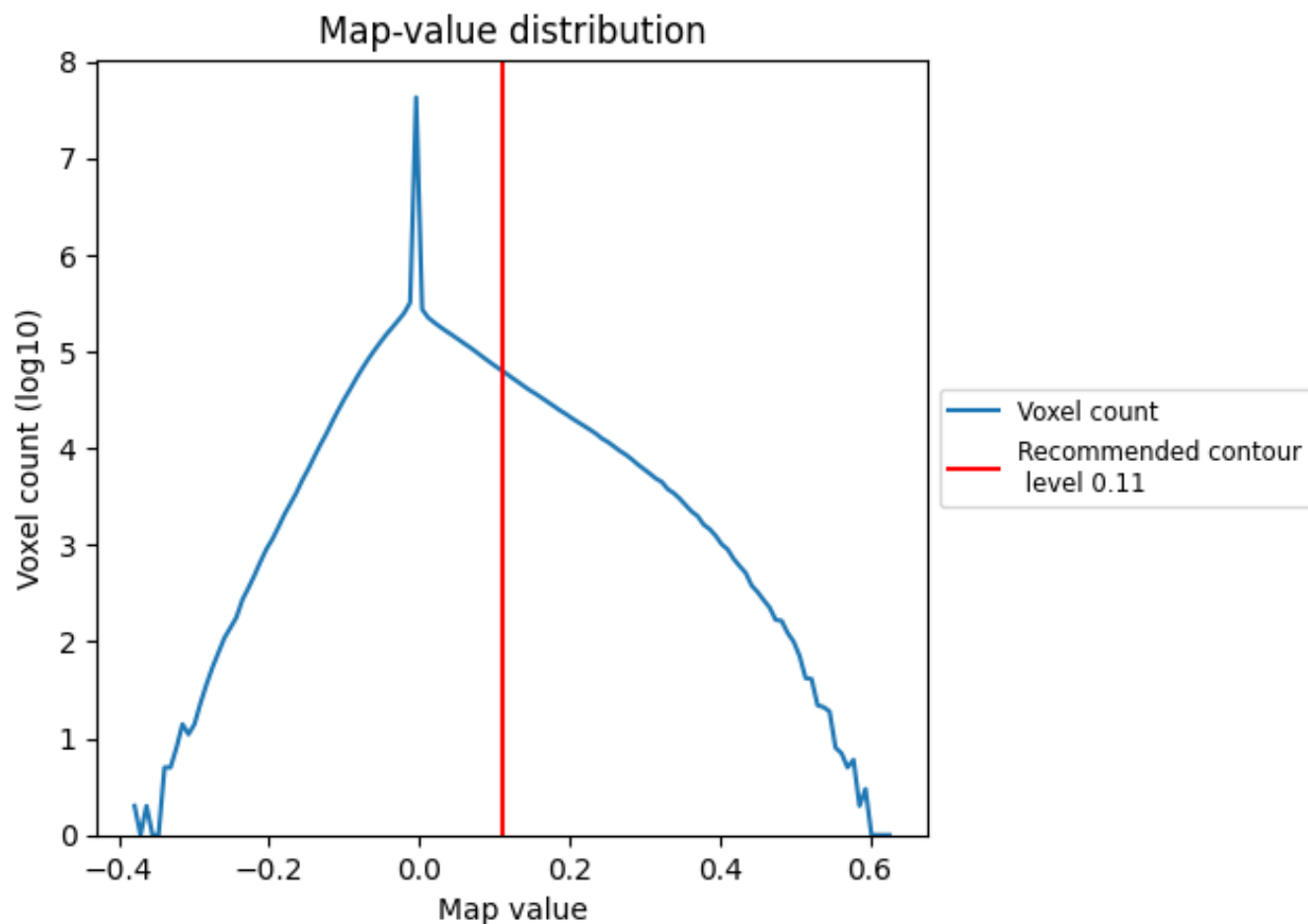
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

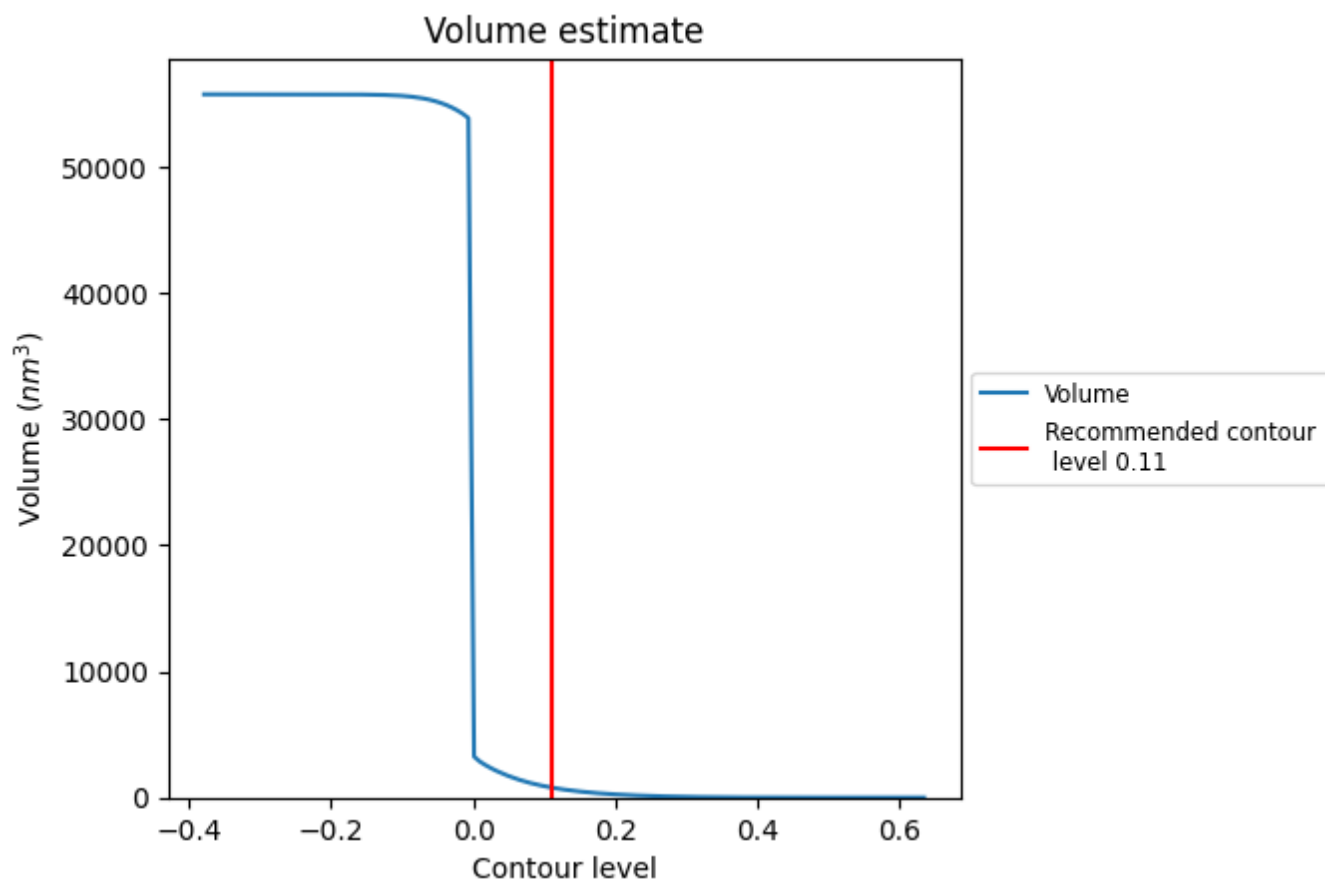
This section contains the results of statistical analysis of the map.

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.

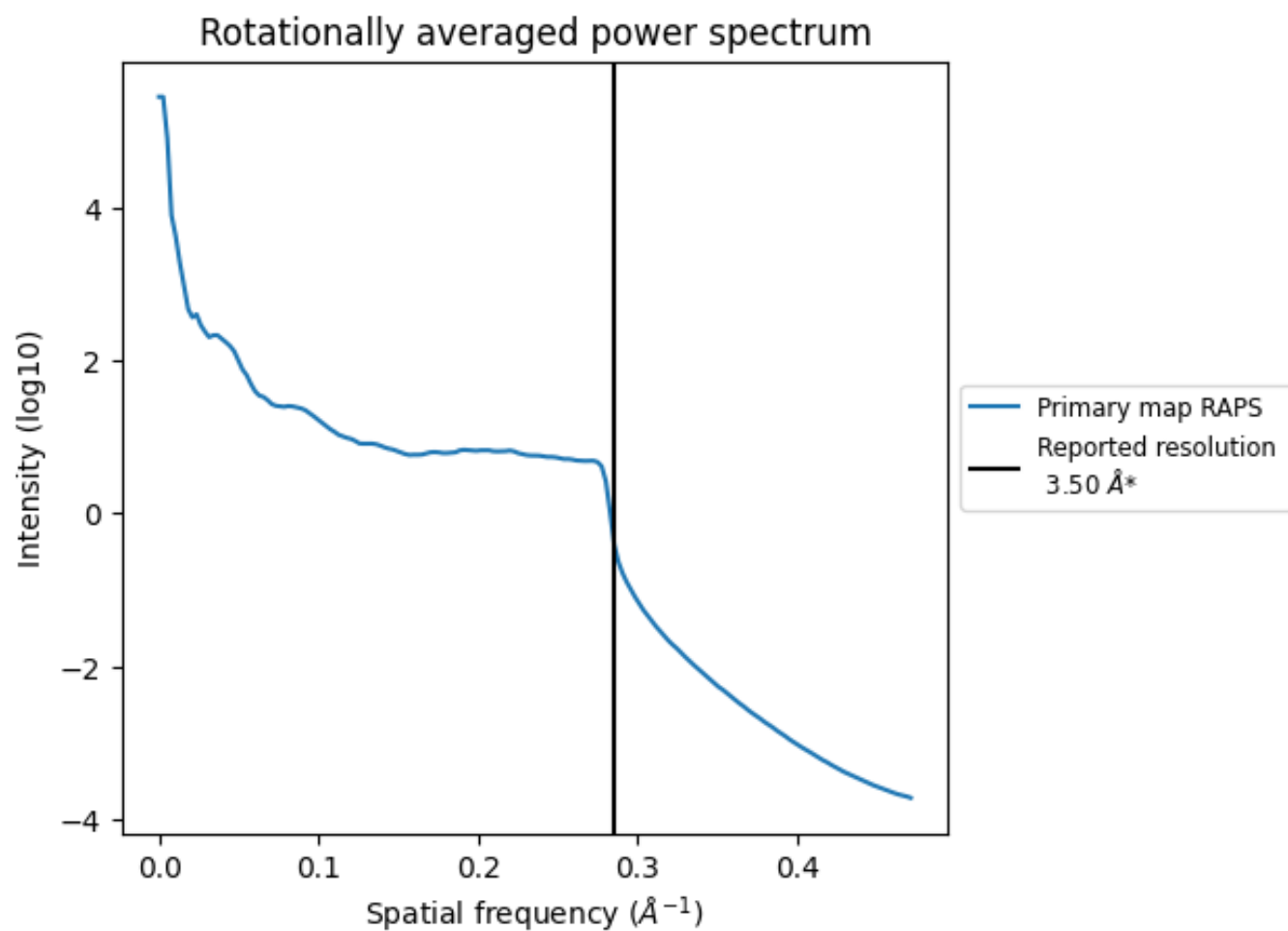
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 793 nm³; this corresponds to an approximate mass of 716 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

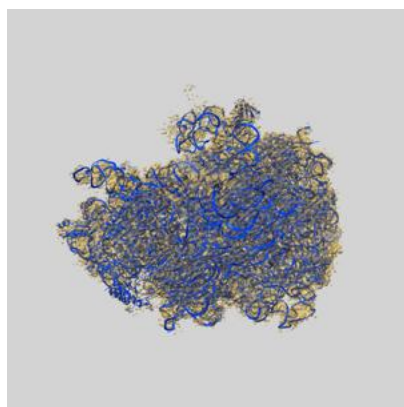
8 Fourier-Shell correlation

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

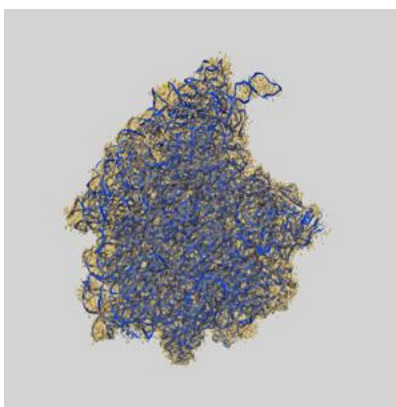
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0177 and PDB model 6HA8. Per-residue inclusion information can be found in section [3](#) on page [17](#).

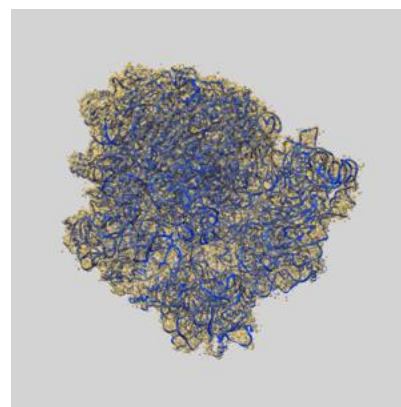
9.1 Map-model overlay [i](#)



X



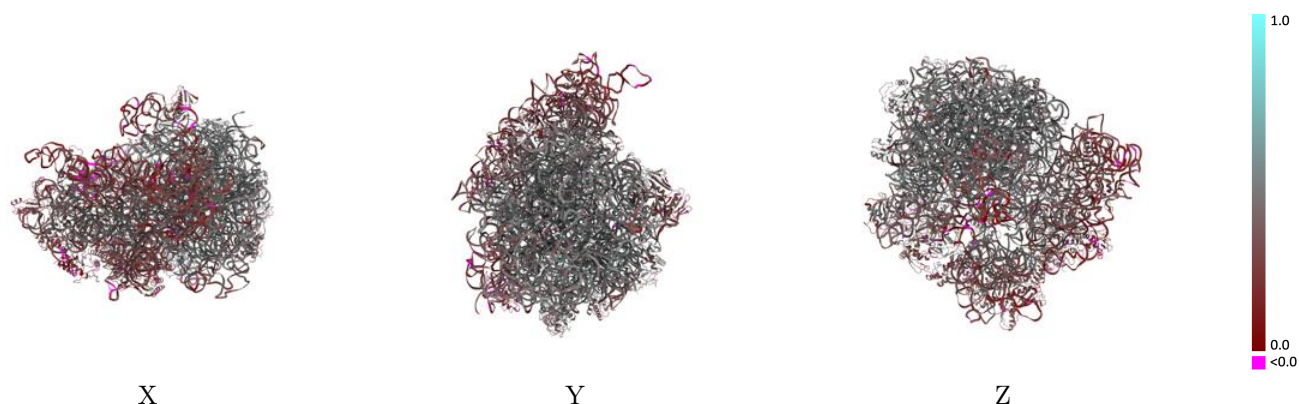
Y



Z

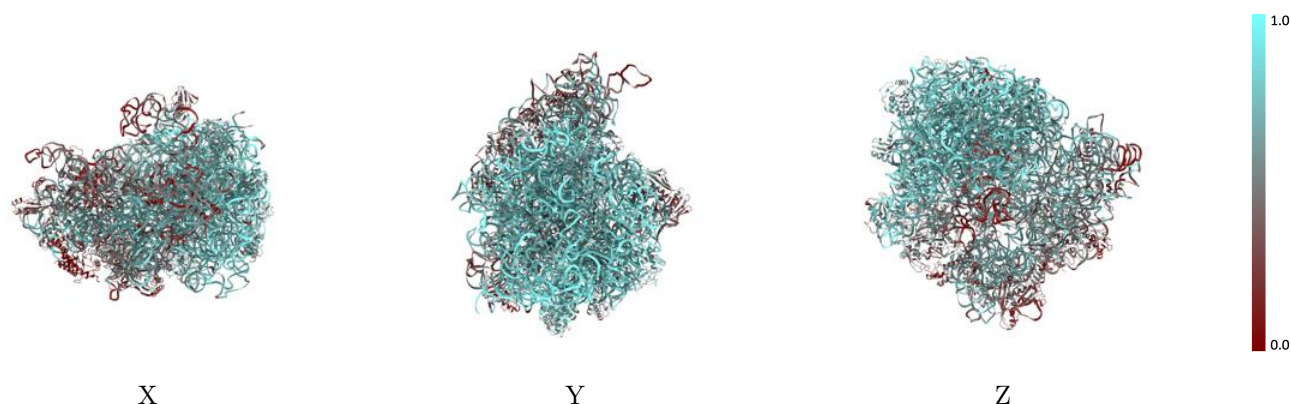
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



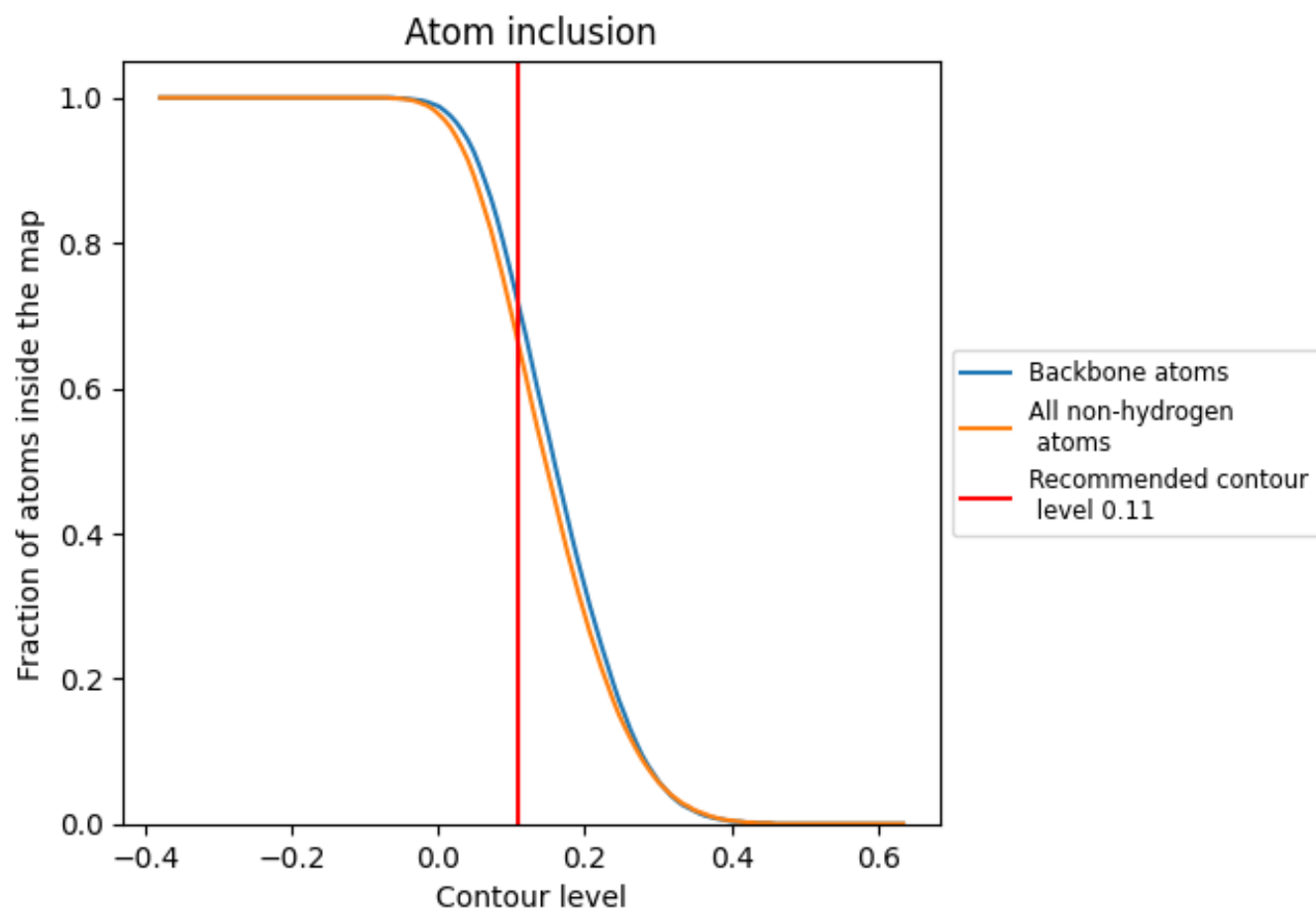
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 66% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6580	 0.3890
0	 0.7190	 0.4870
1	 0.6740	 0.4410
2	 0.7360	 0.5030
3	 0.7260	 0.5080
4	 0.6140	 0.4620
6	 0.2940	 0.2640
7	 0.6670	 0.4050
8	 0.0760	 0.1430
A	 0.7960	 0.4370
B	 0.7850	 0.4020
C	 0.6760	 0.4800
D	 0.6960	 0.4810
E	 0.6820	 0.4500
F	 0.4590	 0.3260
G	 0.4150	 0.3170
J	 0.7100	 0.4720
K	 0.6450	 0.4620
L	 0.6630	 0.4490
M	 0.6350	 0.4500
N	 0.6840	 0.4640
O	 0.5470	 0.3630
P	 0.6320	 0.4500
Q	 0.7070	 0.4500
R	 0.6890	 0.4530
S	 0.7030	 0.4810
T	 0.6140	 0.4430
U	 0.6150	 0.4040
V	 0.4240	 0.3890
W	 0.6490	 0.4500
X	 0.5230	 0.4500
Y	 0.5880	 0.3610
Z	 0.6360	 0.4400
a	 0.6450	 0.3360
b	 0.1210	 0.1970



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Chain	Atom inclusion	Q-score
c	 0.3990	 0.3340
d	 0.2450	 0.2270
e	 0.4970	 0.3750
f	 0.2840	 0.2490
g	 0.4500	 0.3240
h	 0.3960	 0.2870
i	 0.4340	 0.3220
j	 0.3410	 0.3210
k	 0.3790	 0.2970
l	 0.3720	 0.3080
m	 0.3810	 0.2880
n	 0.3810	 0.3480
o	 0.3850	 0.2490
p	 0.3260	 0.2690
q	 0.2850	 0.2390
r	 0.3410	 0.2730
s	 0.3460	 0.2600
t	 0.3710	 0.2630
x	 0.4340	 0.3210