



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 10:07 PM EDT

PDB ID : 5U4I
EMDB ID : EMD-8505
Title : Structural Basis of Co-translational Quality Control by ArfA and RF2 Bound to Ribosome
Authors : Zeng, F.; Chen, Y.; Remis, J.; Shekhar, M.; Phillips, J.C.; Tajkhorshid, E.; Jin, H.
Deposited on : 2016-12-04
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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

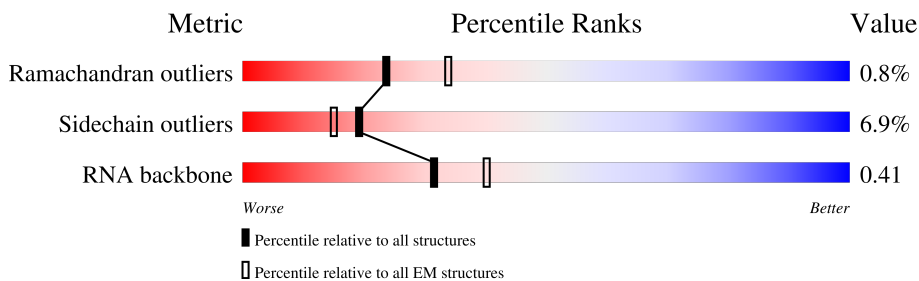
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)
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	2904	30% (Poor fit) 69% (0 outliers) 31% (1 outlier)
2	B	118	66% (0 outliers) 70% (1 outlier) 30% (2 outliers)
3	C	273	70% (0 outliers) 92% (1 outlier) 8% (2 outliers)
4	D	209	86% (0 outliers) 94% (1 outlier) 6% (2 outliers)
5	E	201	79% (0 outliers) 96% (1 outlier) . (2 outliers)
6	F	179	93% (0 outliers) 90% (1 outlier) 9% (2 outliers)
7	G	177	96% (0 outliers) 97% (1 outlier) .. (2 outliers)
8	H	149	100% (0 outliers) 95% (1 outlier) 5% (2 outliers)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	142	99% 91% 8%
10	K	142	96% 99%
11	L	123	82% 93% 7%
12	M	144	92% 94% 6%
13	N	136	85% 96%
14	O	127	85% 90% 5% 6%
15	P	117	94% 91% 8%
16	Q	115	96% 94% 5%
17	R	118	84% 92% 7%
18	S	103	83% 95%
19	T	110	48% 98%
20	U	100	81% 89% 7%
21	V	104	83% 92% 6%
22	W	94	96% 90% 10%
23	X	85	87% 85% 6% 9%
24	Y	78	97% 90% 9%
25	Z	63	84% 94% 5%
26	0	59	83% 95%
27	1	57	75% 95%
28	2	55	89% 87% 9%
29	3	46	70% 100%
30	4	65	98% 98%
31	5	38	100% 100%
32	a	1533	40% 68% 32%
33	b	241	85% 87% 6% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	c	233	69% 80% 8% 12%
35	d	206	96% 92% 7%
36	e	167	69% 86% 8% 6%
37	f	135	67% 70% 26%
38	g	179	76% 80% 16%
39	h	129	88% 95% 5%
40	i	130	88% 88% 10%
41	j	103	91% 83% 13% 5%
42	k	117	91% 97%
43	l	123	68% 93% 7%
44	m	118	92% 91% 5%
45	n	100	93% 93% 7%
46	o	88	73% 88% 13%
47	p	82	98% 90% 10%
48	q	84	86% 87% 8% 5%
49	r	75	83% 81% 5% 13%
50	s	82	94% 90% 9%
51	t	86	100% 95% 5%
52	u	71	73% 76% 21%
53	v	383	77% 85% 8% 7%
54	w	57	60% 68% 14% 18%
55	x	77	16% 71% 27%
55	y	77	97% 77% 23%
56	z	18	17% 28% 6% 67%

2 Entry composition i

There are 58 unique types of molecules in this entry. The entry contains 149495 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
			Total	C	N	O	P		
1	A	2904	62351	27820	11472	20155	2904	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	887	A	U	conflict	GB 42756

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	118	2529	1126	464	821	118	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	77	Total	C	N	O	S	0	0
			588	363	118	106	1		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	2	50	Total	C	N	O	0	0
			409	263	75	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1533	Total	C	N	O	P	0	0
			32906	14683	6036	10654	1533		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	527	A	G	conflict	GB 817573384

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	b	224	1753	1109	315	321	8	0	0

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	d	204	1633	1020	313	296	4	0	0

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	e	157	1156	719	218	213	6	0	0

- Molecule 37 is a protein called 30S ribosomal protein S6.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S8.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

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

- Molecule 41 is a protein called 30S ribosomal protein S10.

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

- Molecule 42 is a protein called 30S ribosomal protein S11.

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

- Molecule 43 is a protein called 30S ribosomal protein S12.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

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

- Molecule 45 is a protein called 30S ribosomal protein S14.

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

- Molecule 46 is a protein called 30S ribosomal protein S15.

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

- Molecule 47 is a protein called 30S ribosomal protein S16.

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

- Molecule 48 is a protein called 30S ribosomal protein S17.

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

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	65	Total	C	N	O	S	0	0
			539	341	100	97	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	15	GLU	ALA	conflict	UNP P0A7T7

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 52 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 53 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	v	357	2836	1744	498	584	10	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-17	HIS	-	expression tag	UNP P07012
v	-16	HIS	-	expression tag	UNP P07012
v	-15	HIS	-	expression tag	UNP P07012
v	-14	HIS	-	expression tag	UNP P07012
v	-13	HIS	-	expression tag	UNP P07012
v	-12	HIS	-	expression tag	UNP P07012
v	-11	SER	-	expression tag	UNP P07012
v	-10	ALA	-	expression tag	UNP P07012
v	-9	ALA	-	expression tag	UNP P07012
v	-8	LEU	-	expression tag	UNP P07012
v	-7	GLU	-	expression tag	UNP P07012
v	-6	VAL	-	expression tag	UNP P07012
v	-5	LEU	-	expression tag	UNP P07012
v	-4	PHE	-	expression tag	UNP P07012
v	-3	GLN	-	expression tag	UNP P07012
v	-2	GLY	-	expression tag	UNP P07012
v	-1	PRO	-	expression tag	UNP P07012
v	0	GLY	-	expression tag	UNP P07012

- Molecule 54 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	w	47	388	239	82	66	1	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
w	-1	GLY	-	expression tag	UNP P36675
w	0	SER	-	expression tag	UNP P36675

- Molecule 55 is a RNA chain called P-site or E-site fMet-tRNA(fMet).

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

Continued on next page...

Continued from previous page...

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

- Molecule 56 is a RNA chain called mRNA.

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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	100	Total	Mg	0
			100	100	
57	B	4	Total	Mg	0
			4	4	
57	a	20	Total	Mg	0
			20	20	

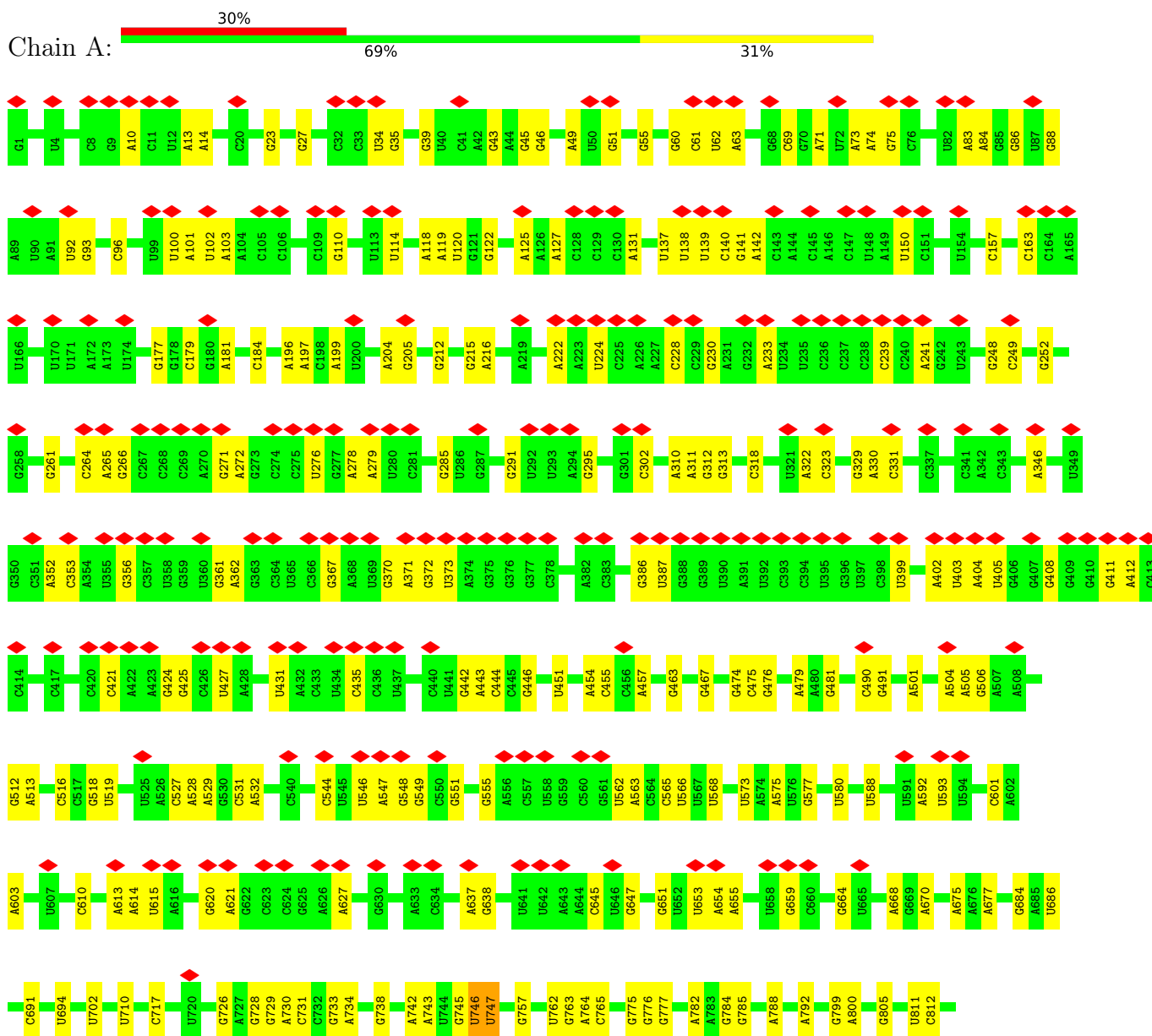
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

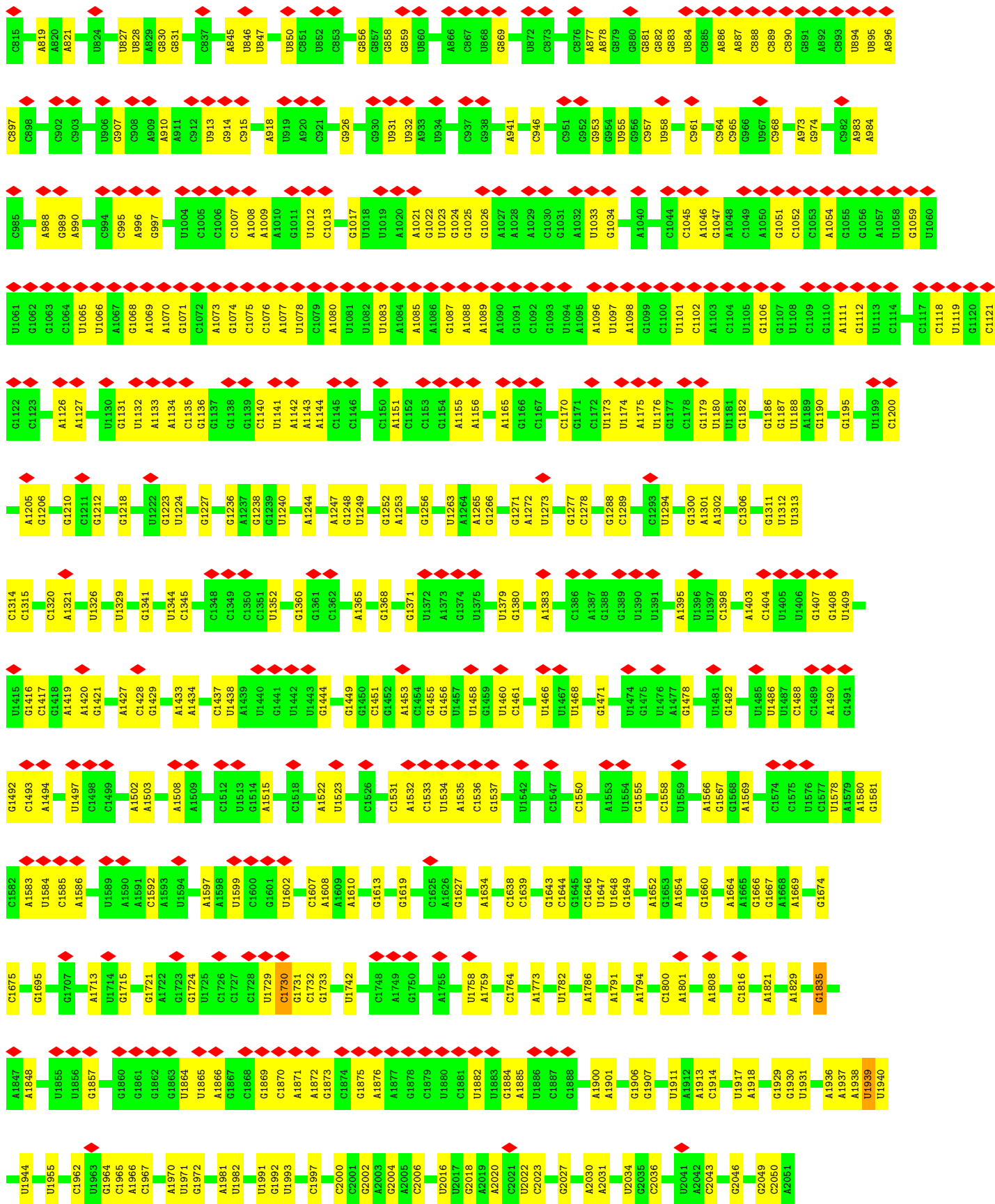
Mol	Chain	Residues	Atoms		AltConf
58	5	1	Total	Zn	0
			1	1	

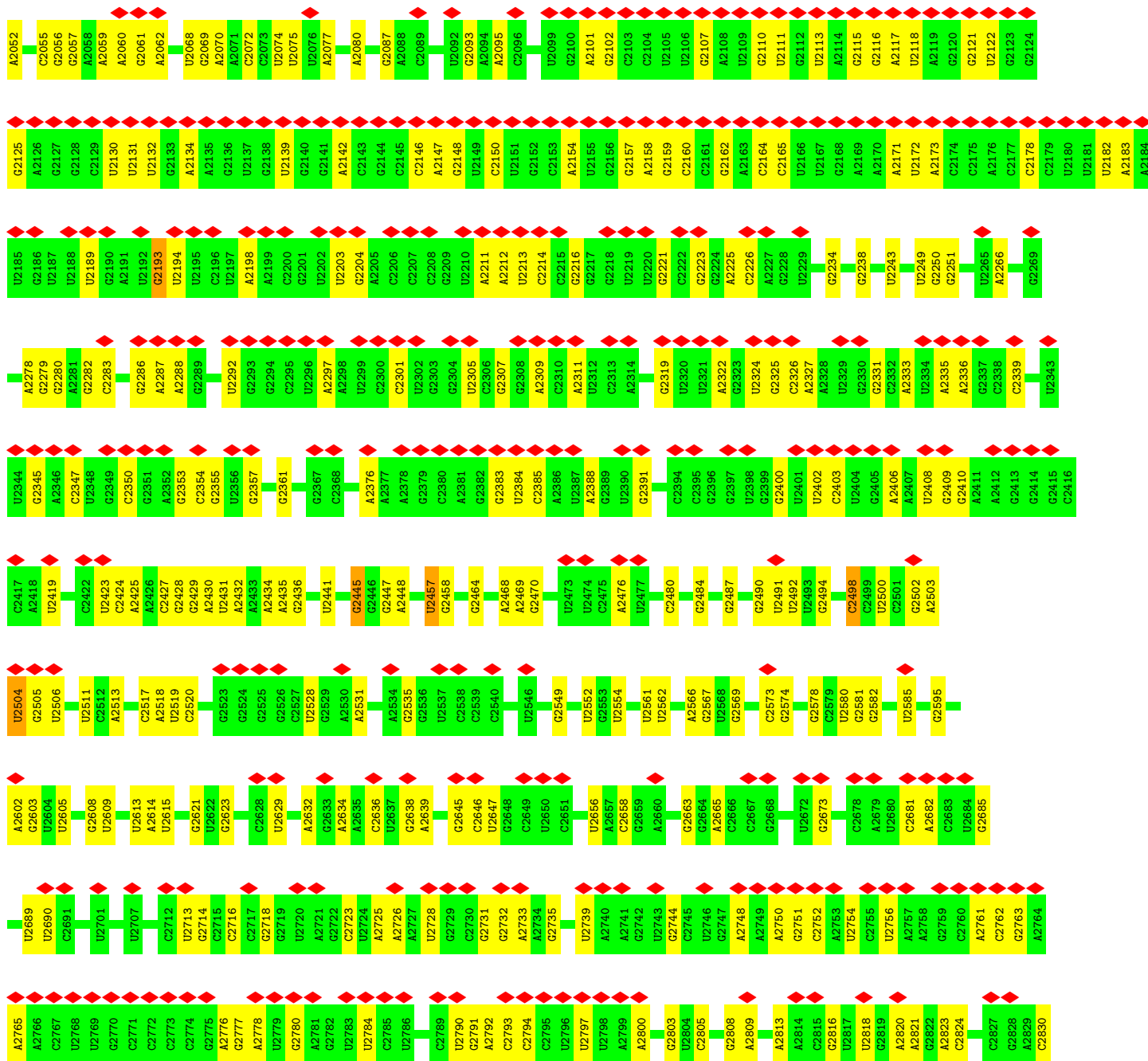
3 Residue-property plots [i](#)

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

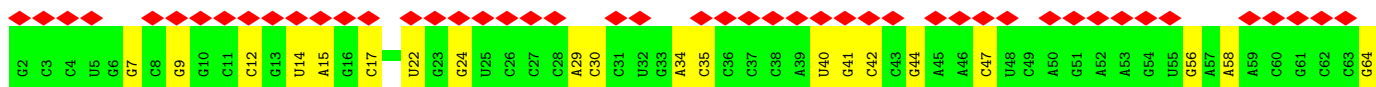
- Molecule 1: 23S rRNA

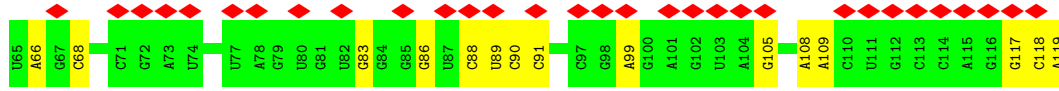




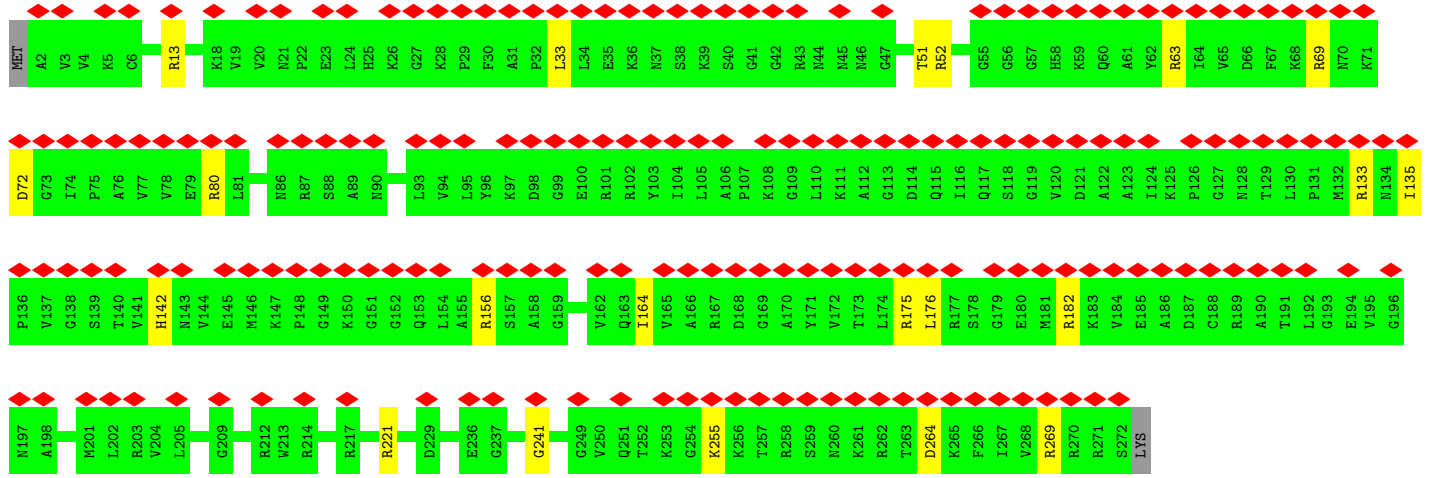
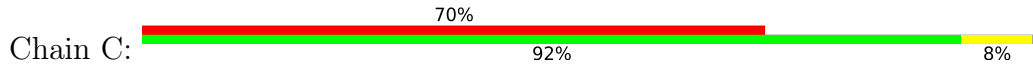


• Molecule 2: 5S rRNA

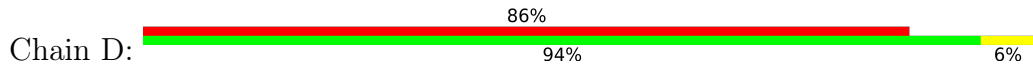




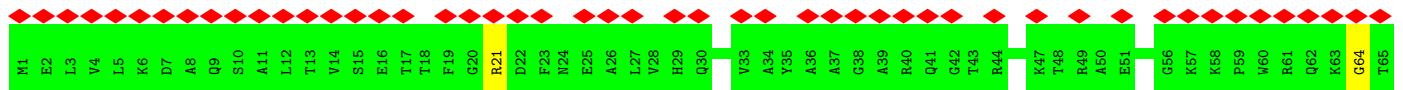
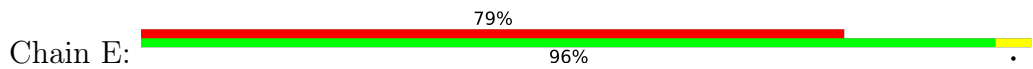
• Molecule 3: 50S ribosomal protein L2

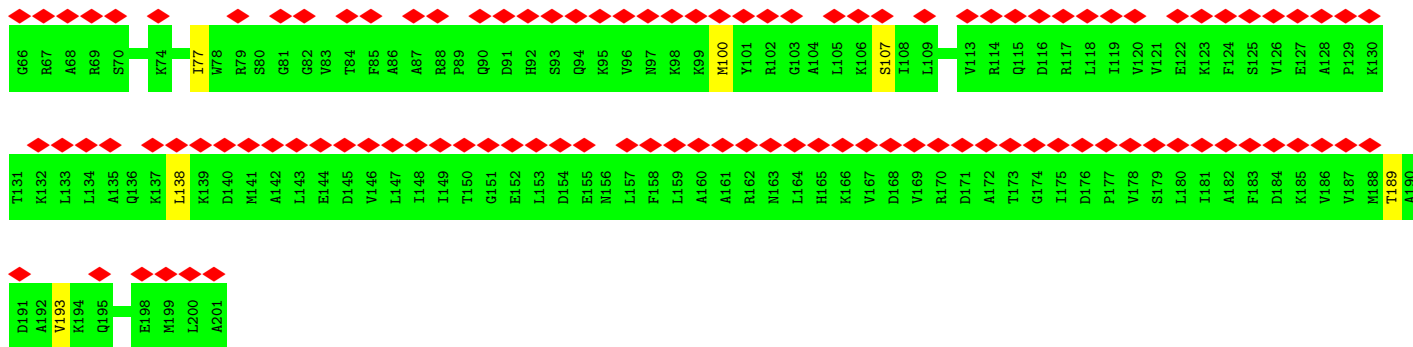


• Molecule 4: 50S ribosomal protein L3

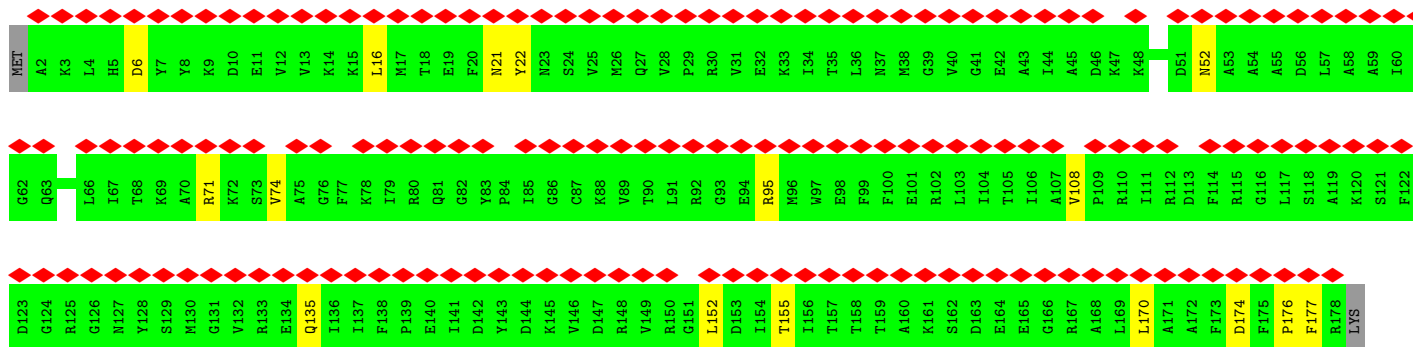
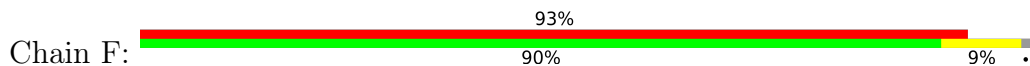


• Molecule 5: 50S ribosomal protein L4

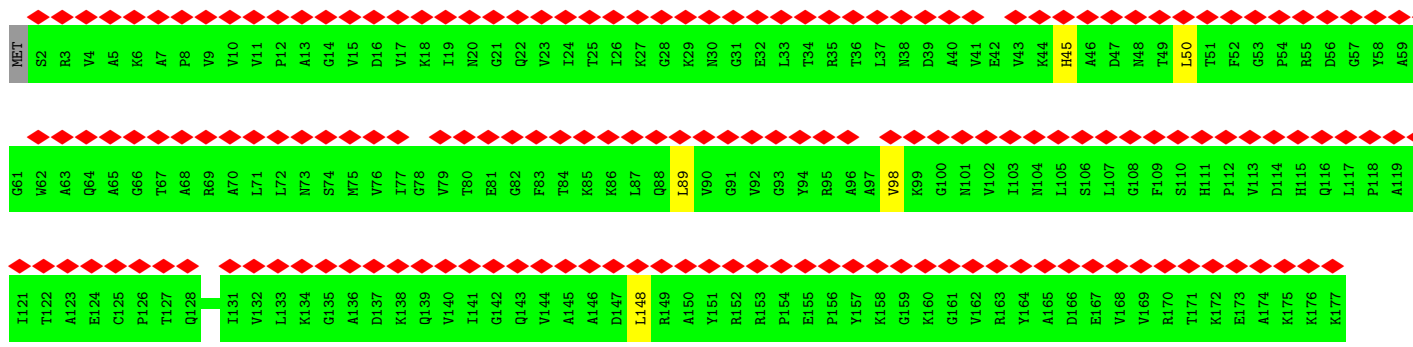




• Molecule 6: 50S ribosomal protein L5

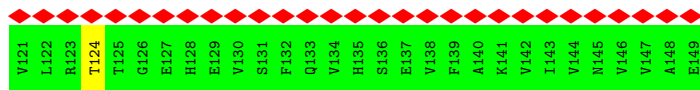


• Molecule 7: 50S ribosomal protein L6

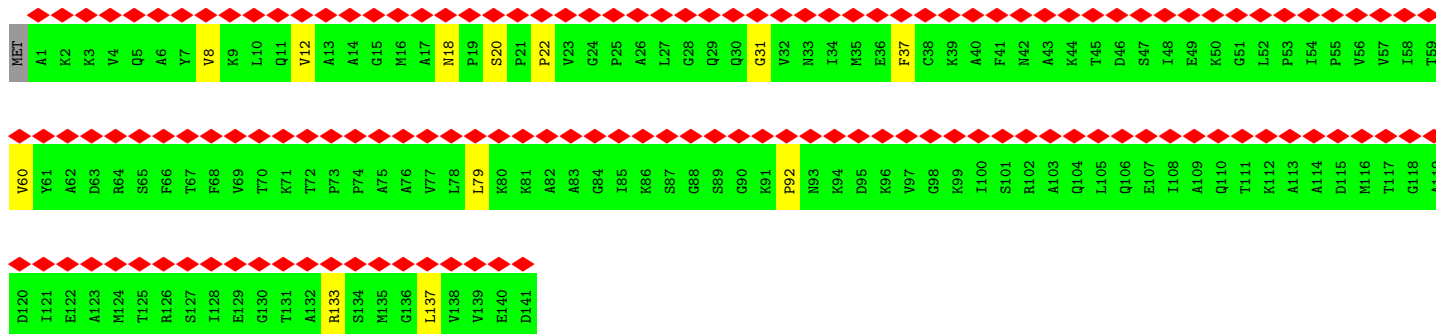
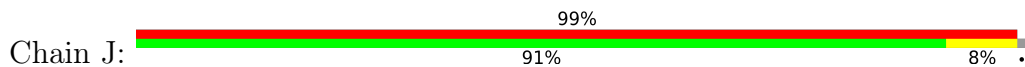


• Molecule 8: 50S ribosomal protein L9

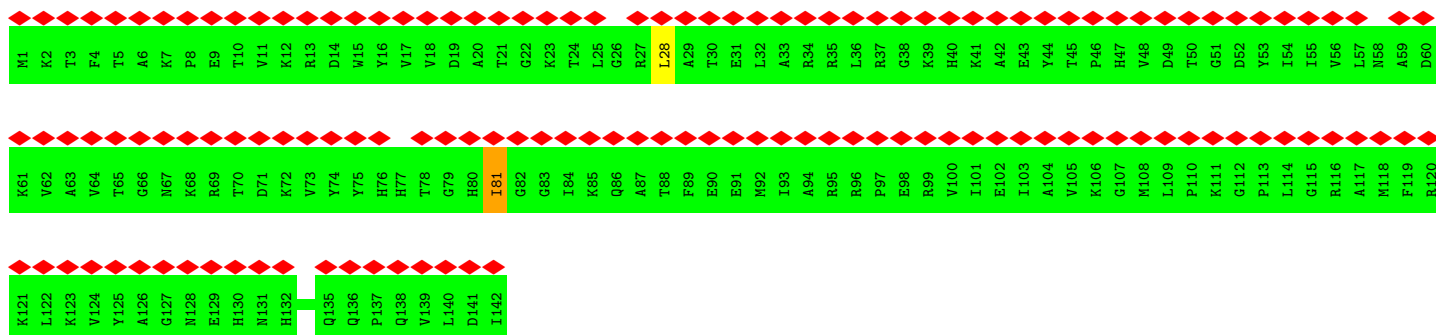




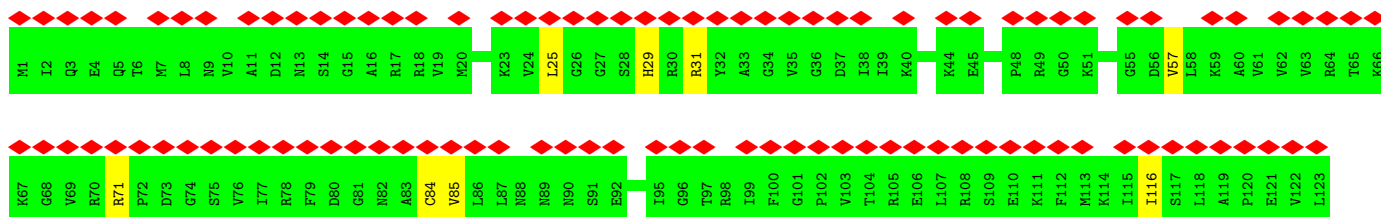
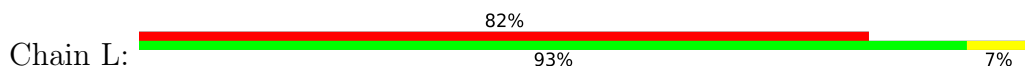
• Molecule 9: 50S ribosomal protein L11



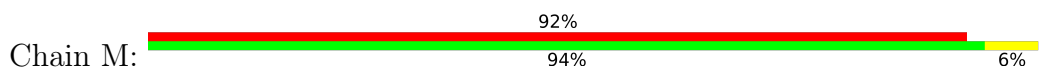
• Molecule 10: 50S ribosomal protein L13

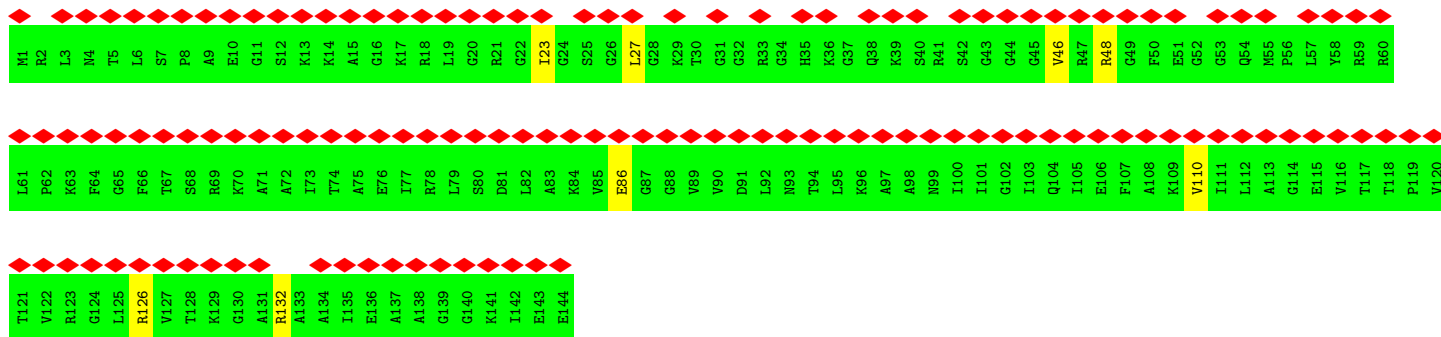


• Molecule 11: 50S ribosomal protein L14

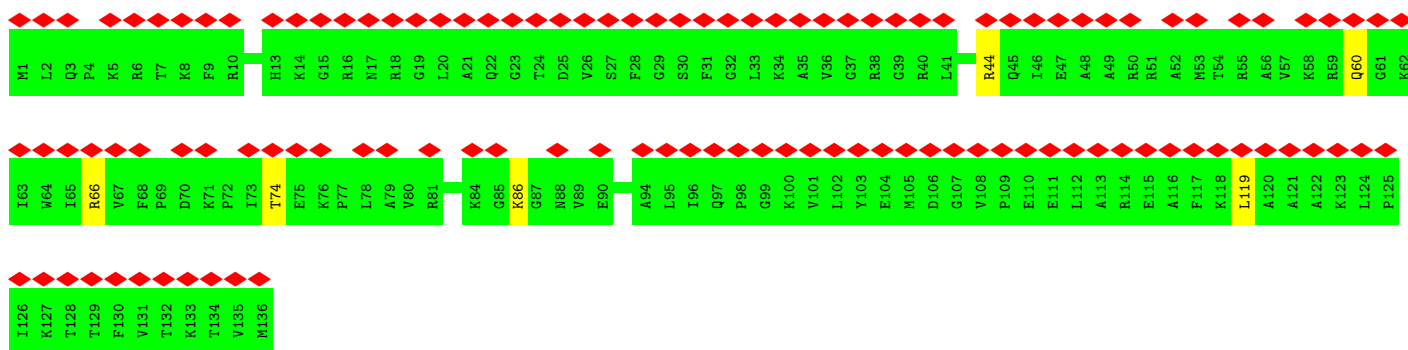
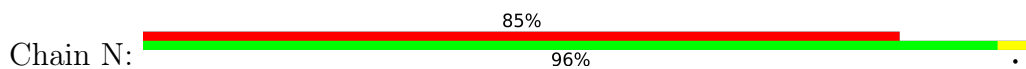


• Molecule 12: 50S ribosomal protein L15

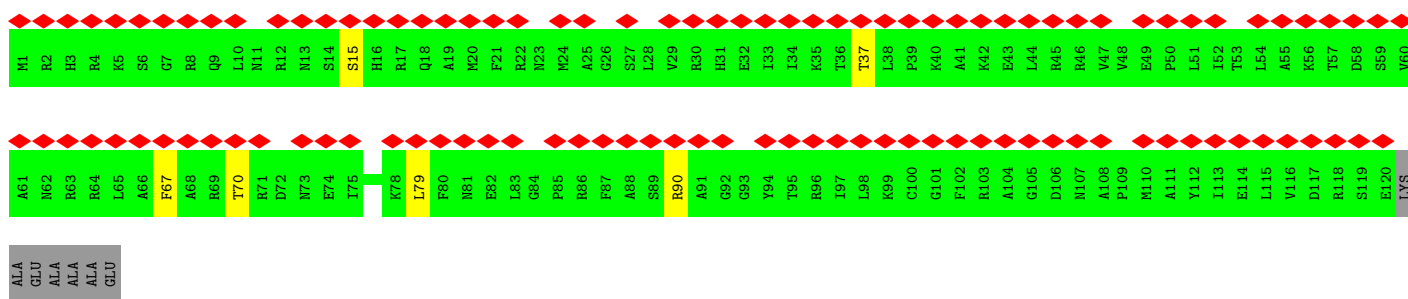
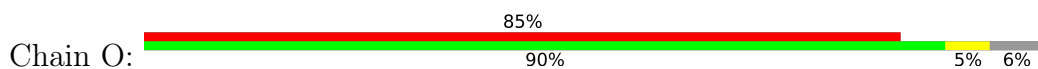




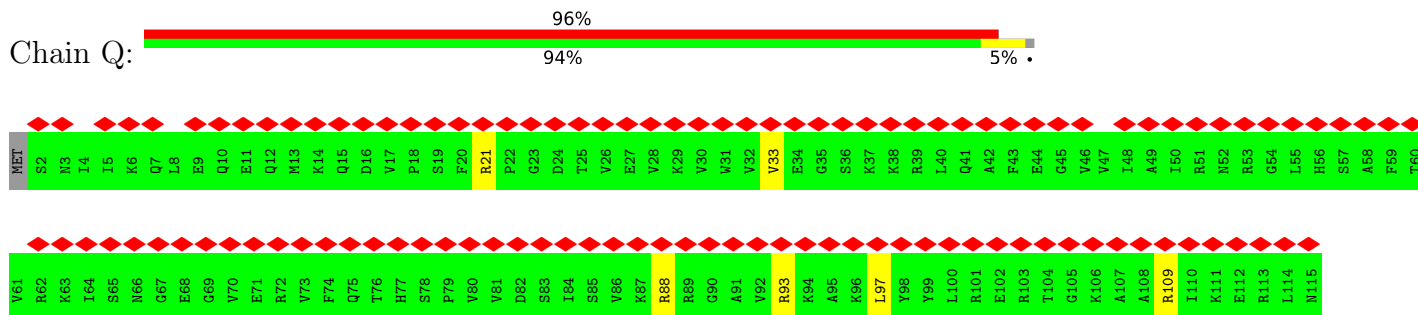
• Molecule 13: 50S ribosomal protein L16



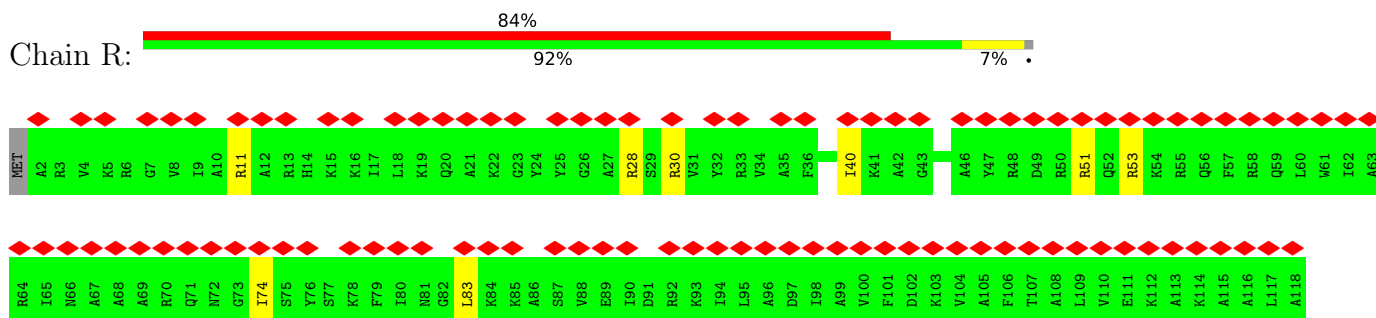
• Molecule 14: 50S ribosomal protein L17



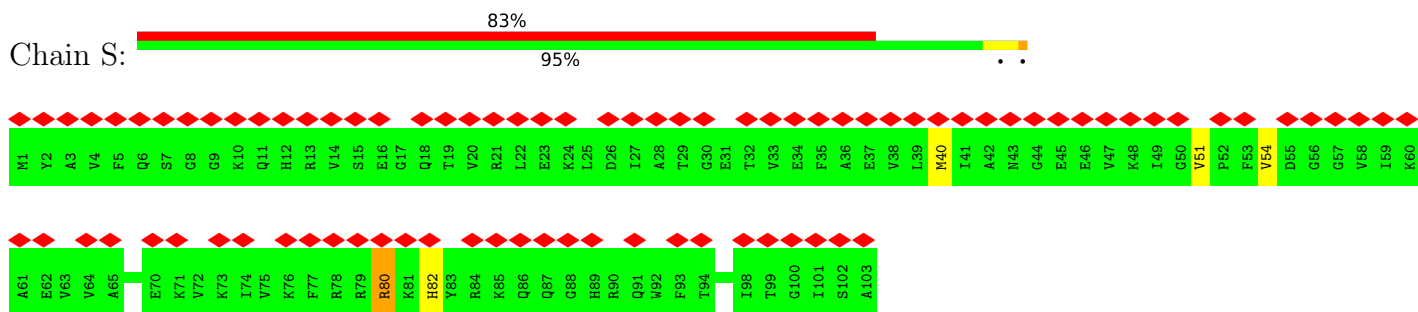
• Molecule 16: 50S ribosomal protein L19



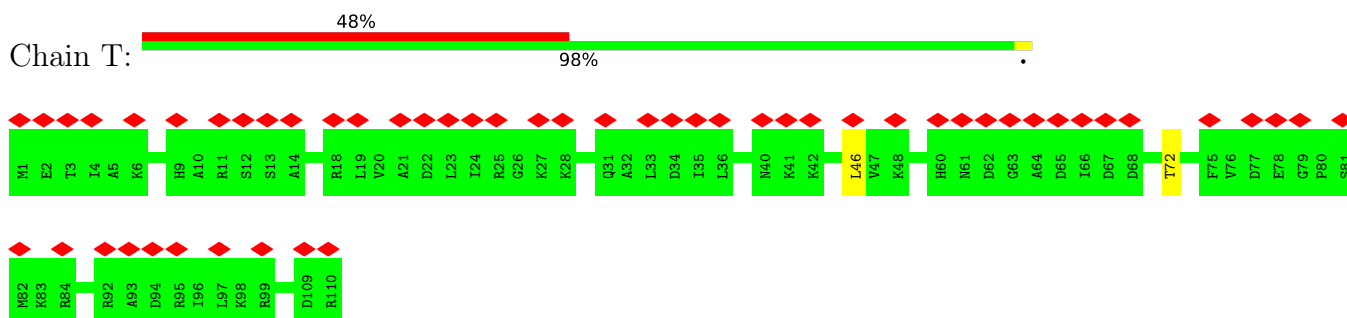
• Molecule 17: 50S ribosomal protein L20



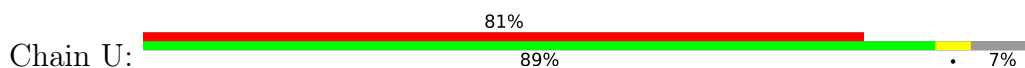
• Molecule 18: 50S ribosomal protein L21

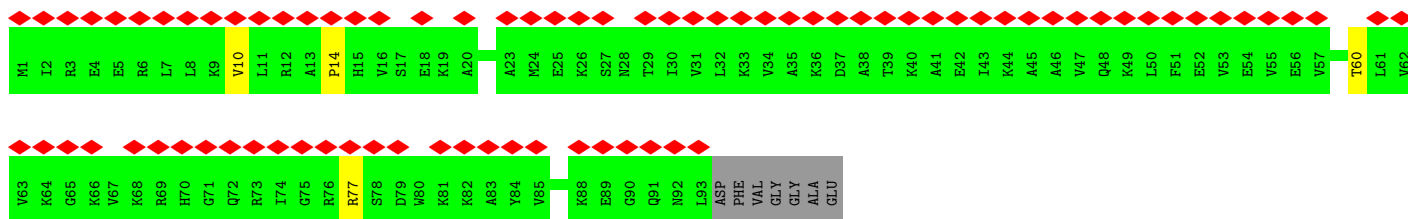


• Molecule 19: 50S ribosomal protein L22

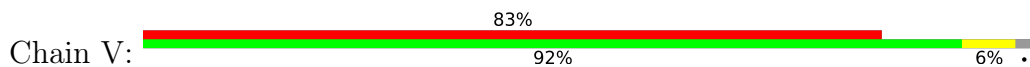


• Molecule 20: 50S ribosomal protein L23

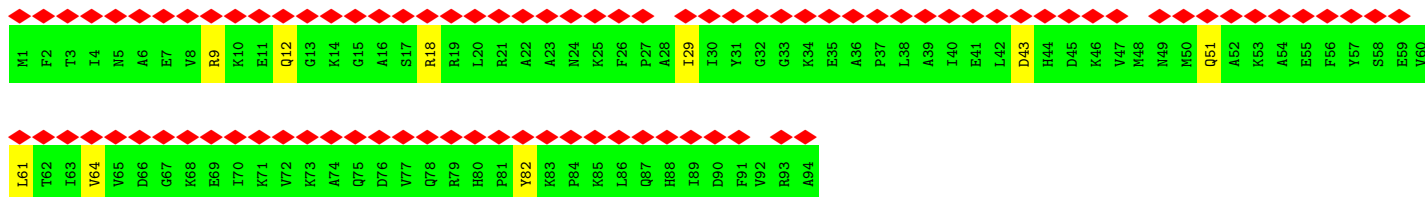
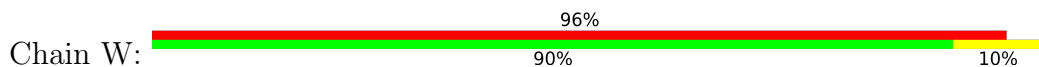




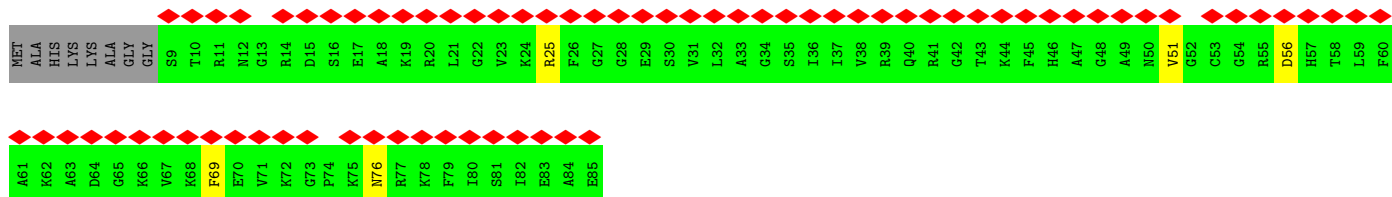
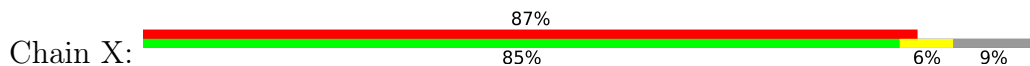
• Molecule 21: 50S ribosomal protein L24



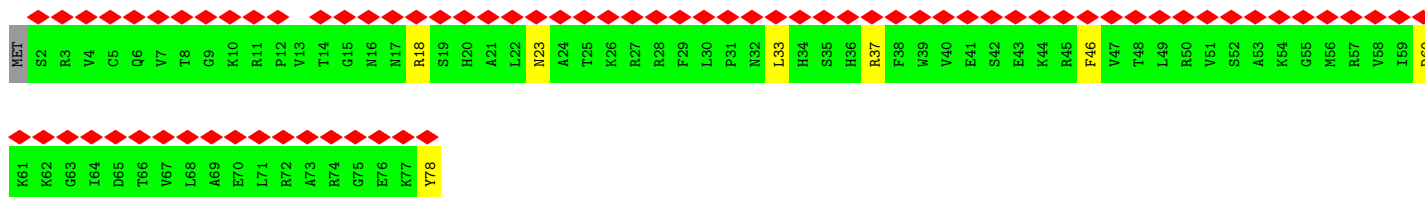
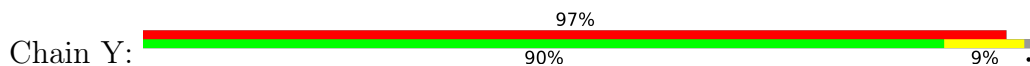
• Molecule 22: 50S ribosomal protein L25



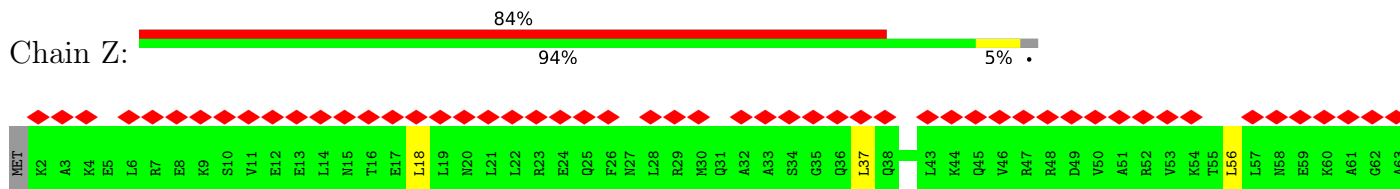
• Molecule 23: 50S ribosomal protein L27



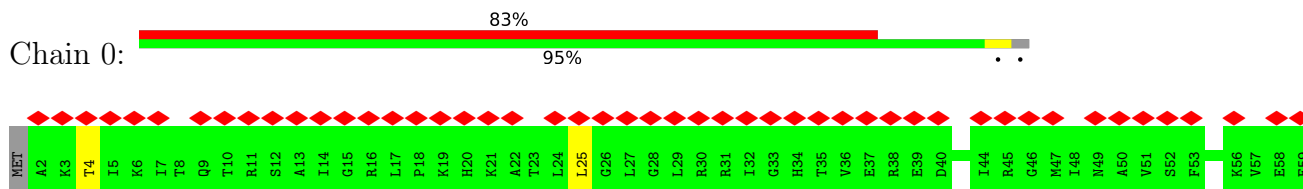
• Molecule 24: 50S ribosomal protein L28



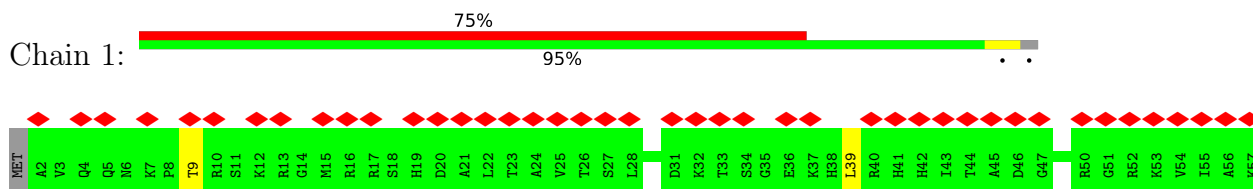
• Molecule 25: 50S ribosomal protein L29



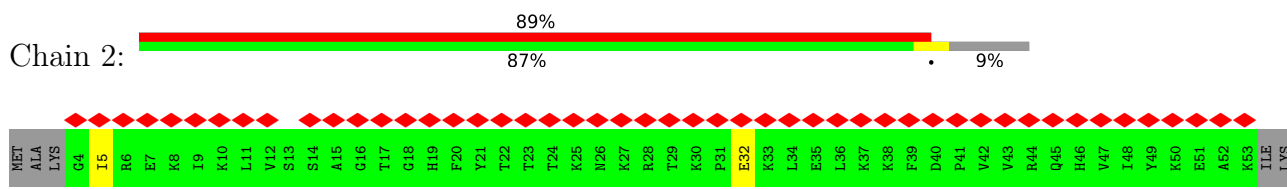
• Molecule 26: 50S ribosomal protein L30



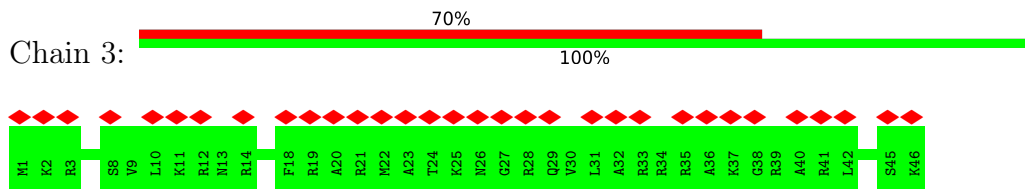
• Molecule 27: 50S ribosomal protein L32



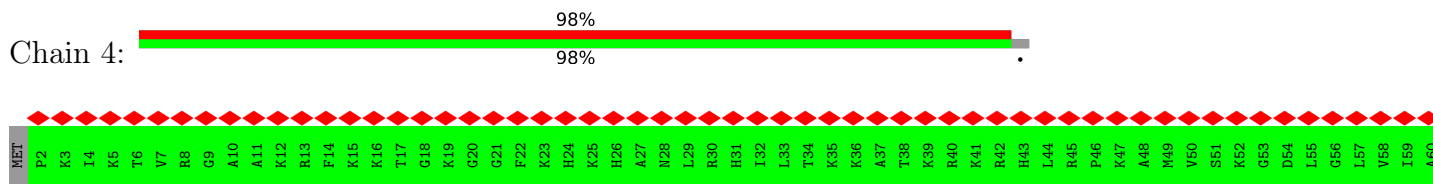
• Molecule 28: 50S ribosomal protein L33



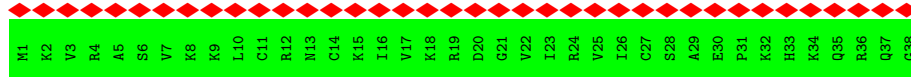
• Molecule 29: 50S ribosomal protein L34



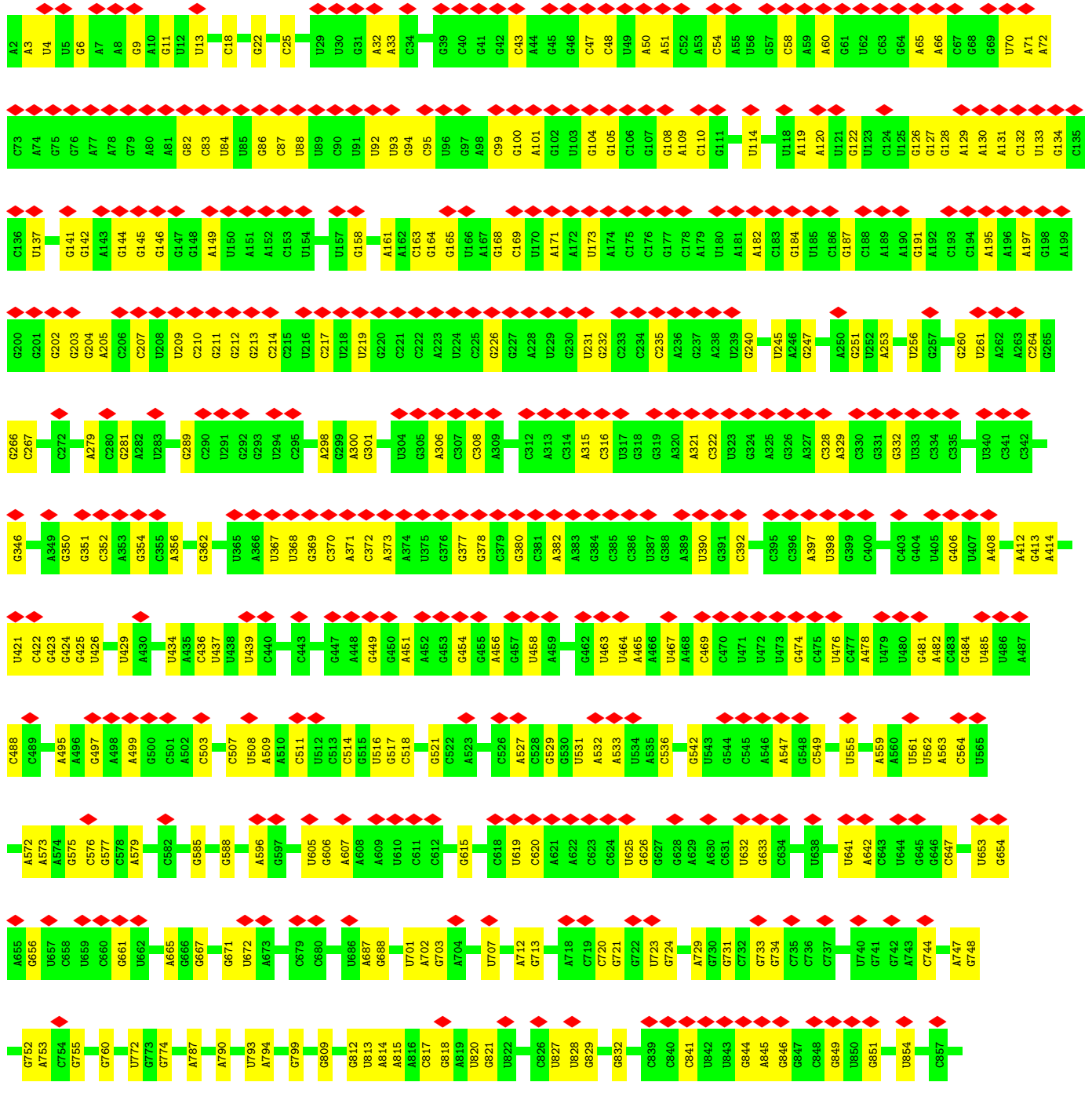
• Molecule 30: 50S ribosomal protein L35

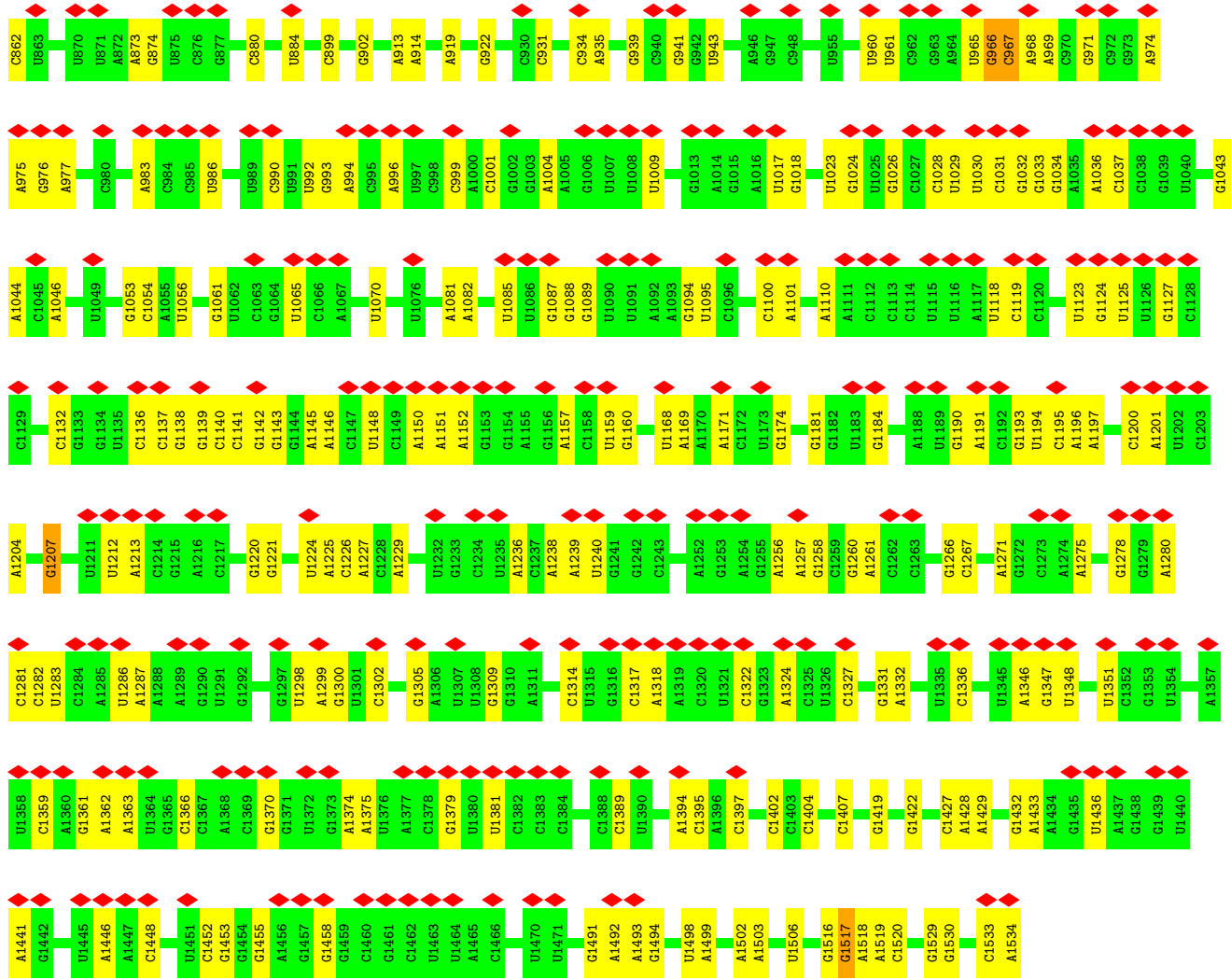


• Molecule 31: 50S ribosomal protein L36

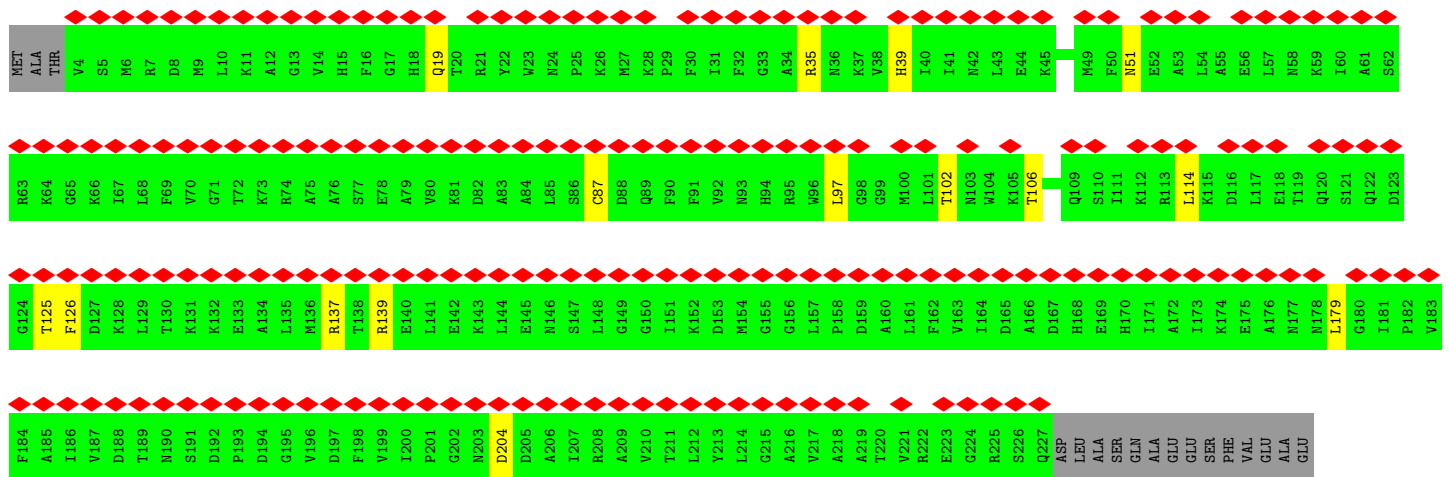
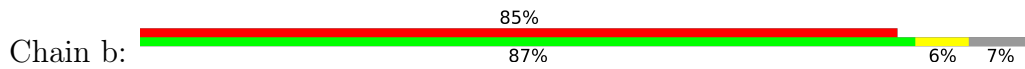


• Molecule 32: 16S rRNA

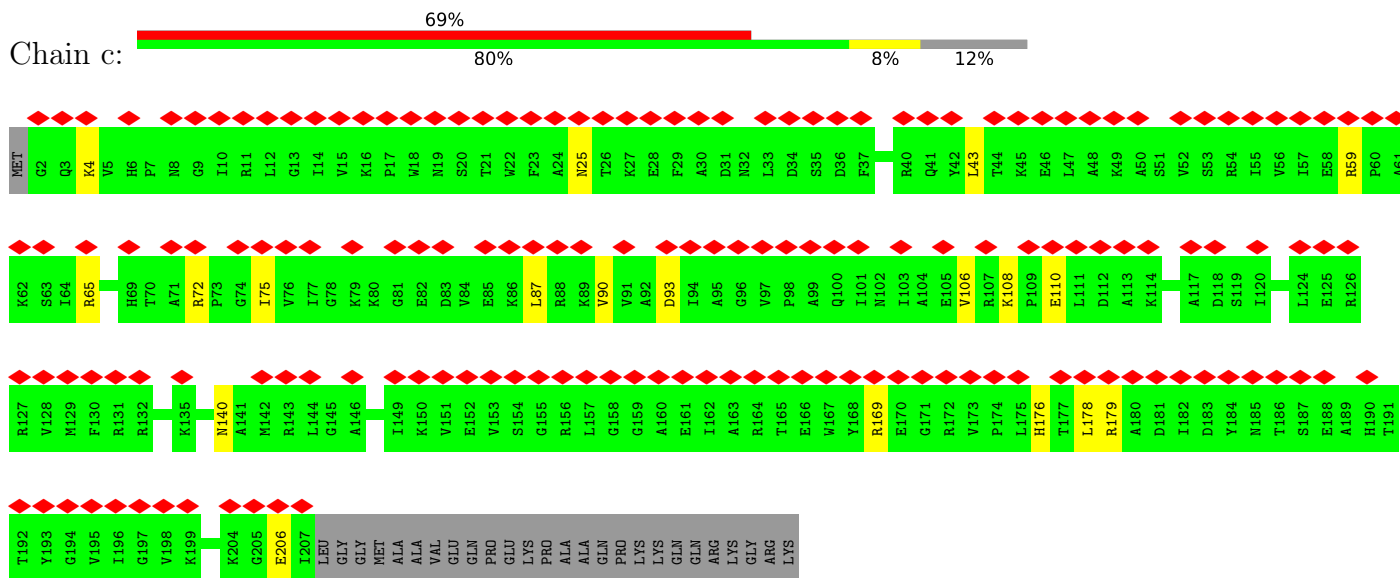




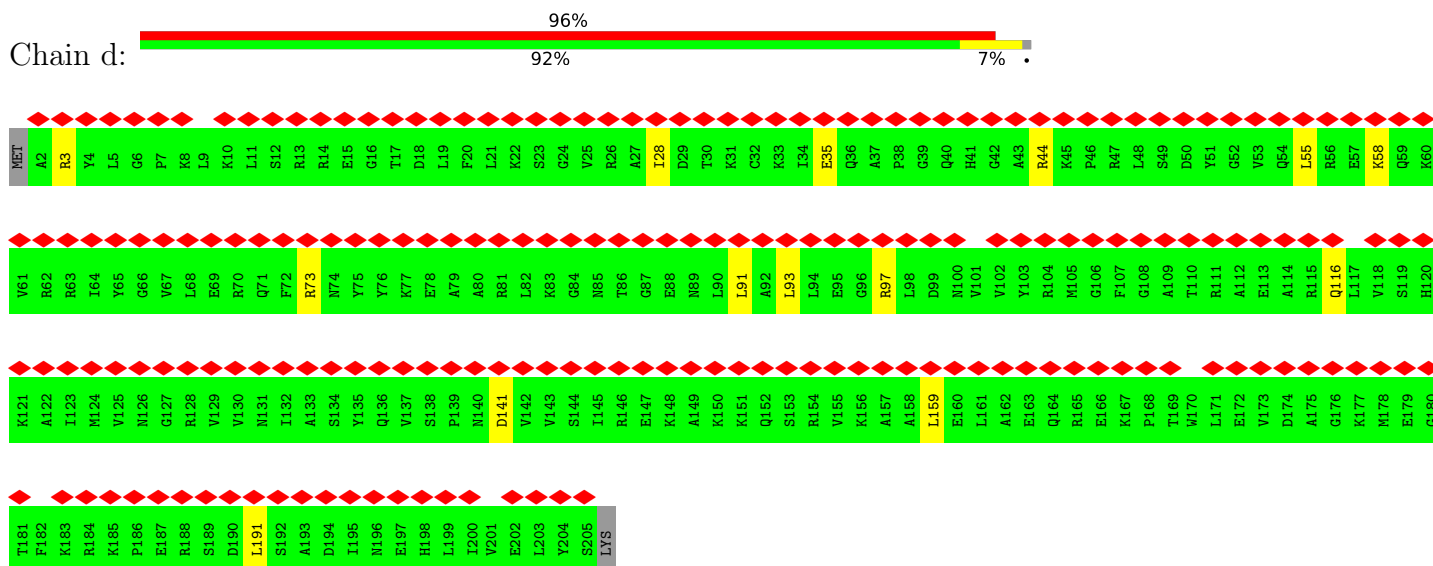
- Molecule 33: 30S ribosomal protein S2



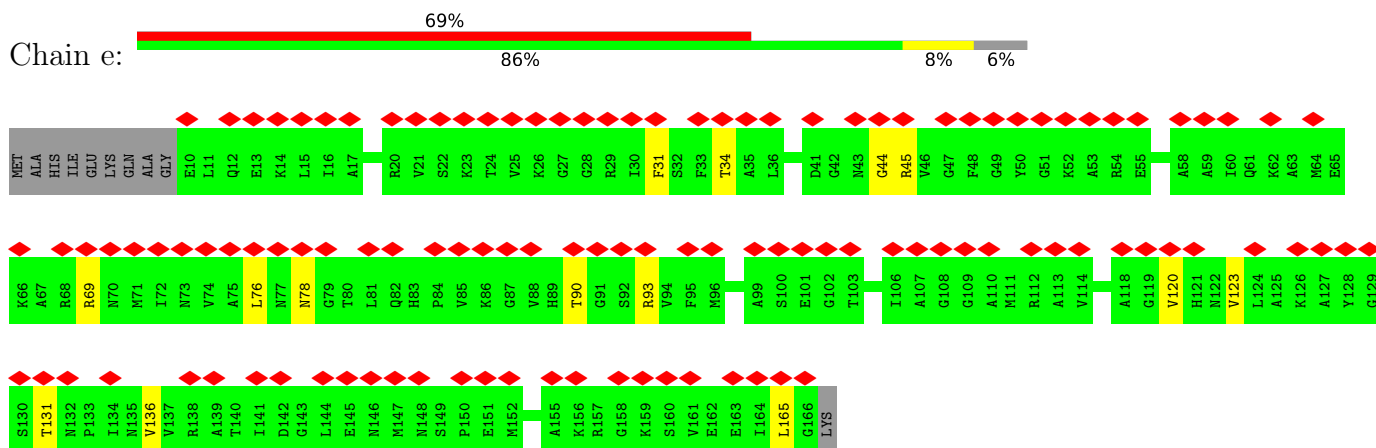
- Molecule 34: 30S ribosomal protein S3



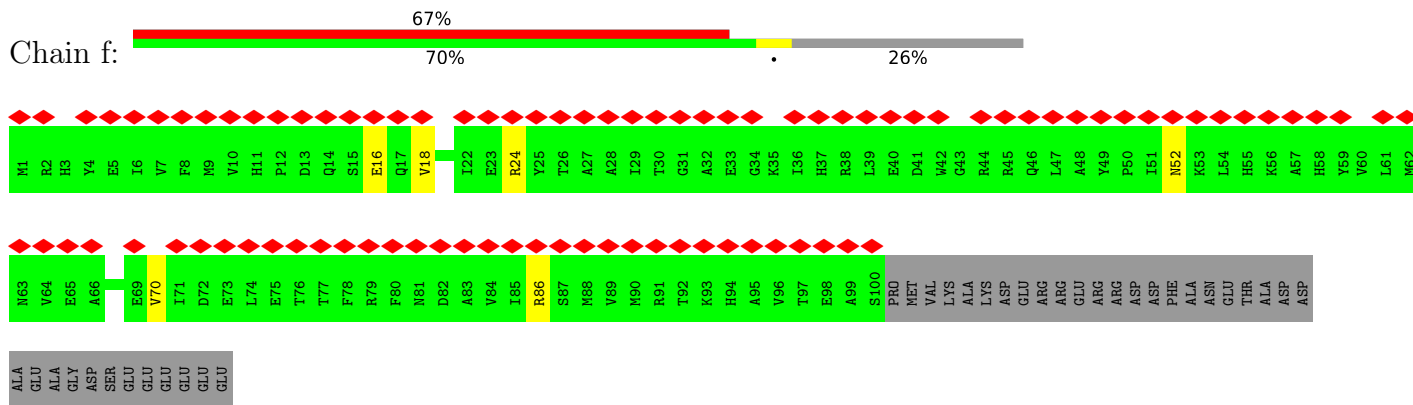
• Molecule 35: 30S ribosomal protein S4



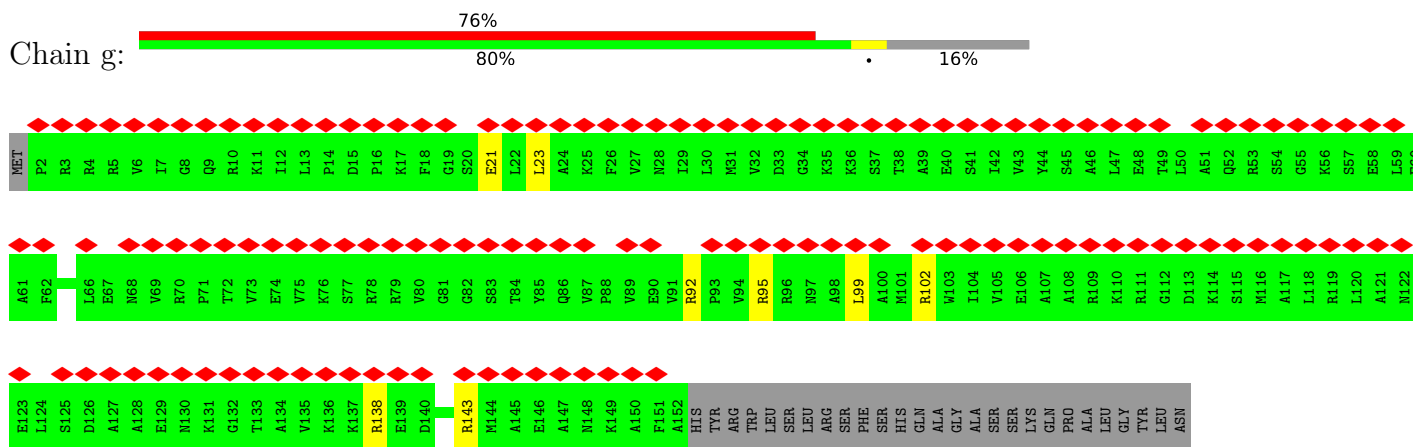
• Molecule 36: 30S ribosomal protein S5



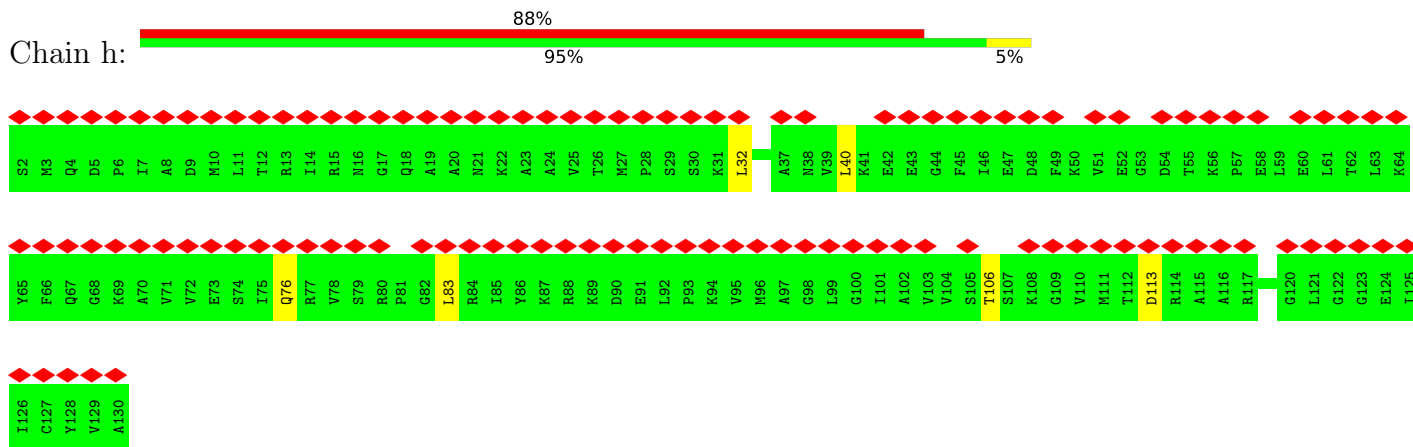
• Molecule 37: 30S ribosomal protein S6



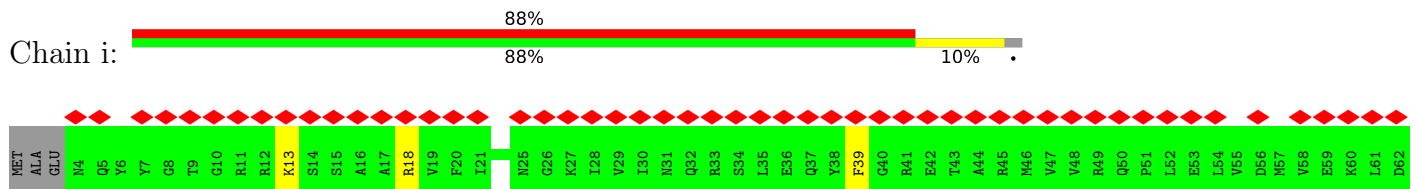
• Molecule 38: 30S ribosomal protein S7

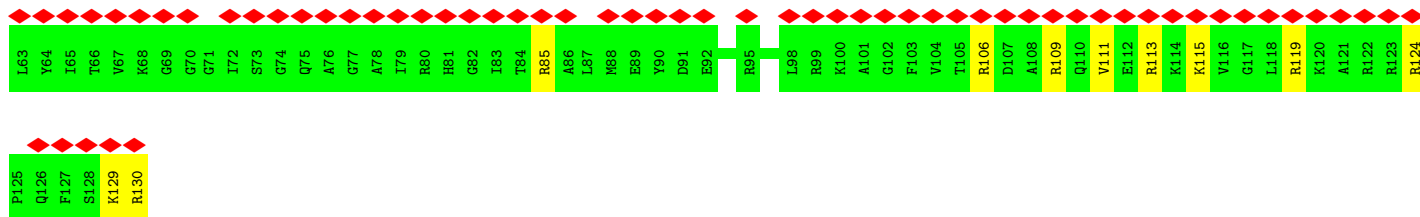


• Molecule 39: 30S ribosomal protein S8

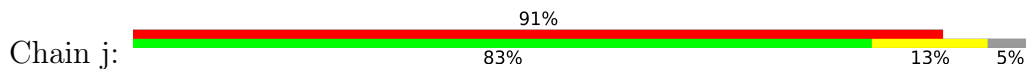


• Molecule 40: 30S ribosomal protein S9

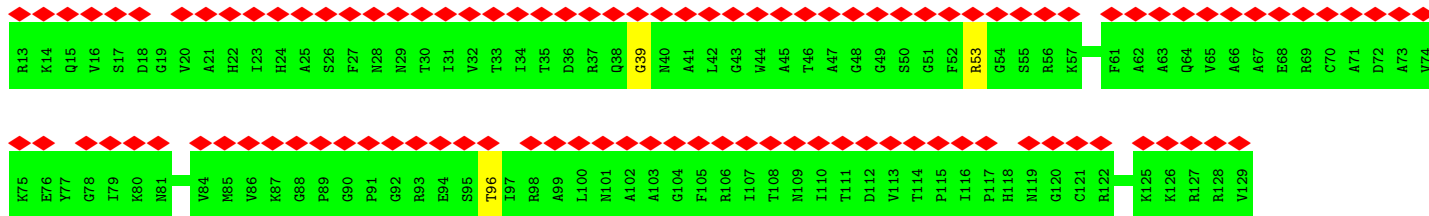




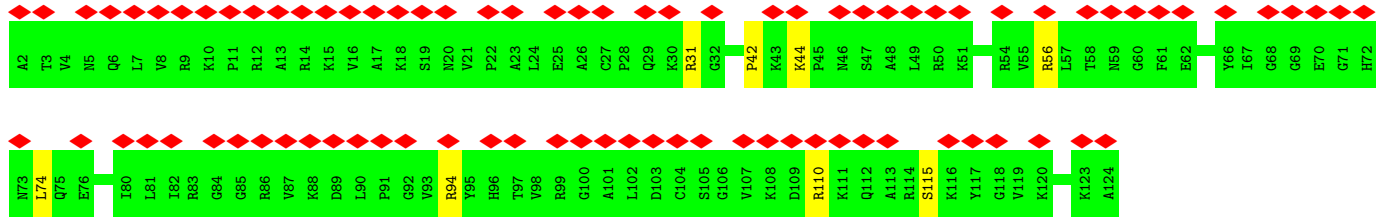
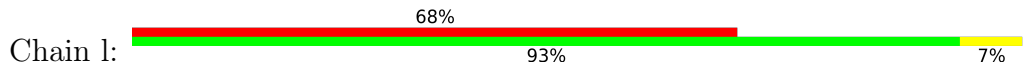
• Molecule 41: 30S ribosomal protein S10



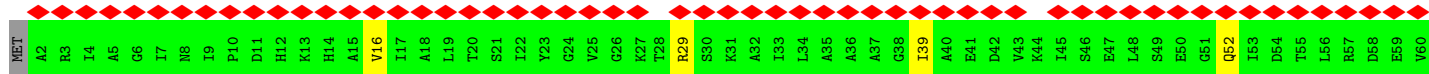
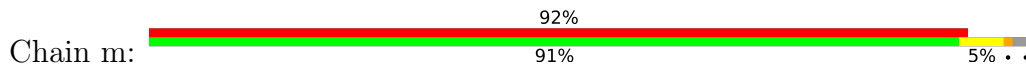
• Molecule 42: 30S ribosomal protein S11

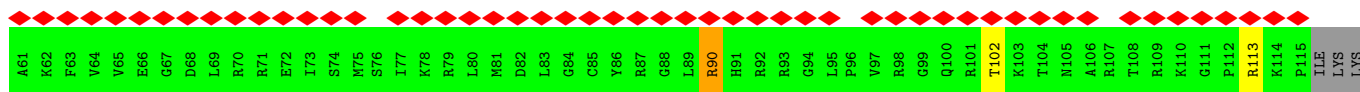


• Molecule 43: 30S ribosomal protein S12

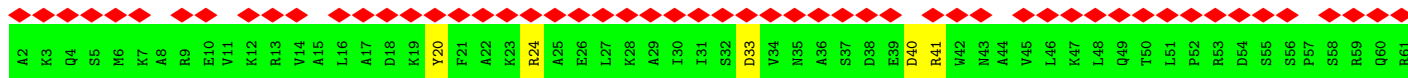
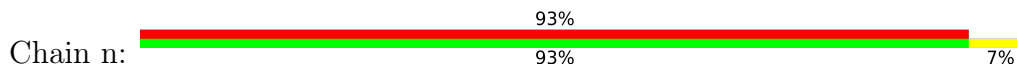


• Molecule 44: 30S ribosomal protein S13

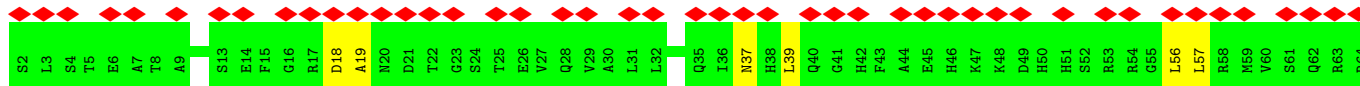
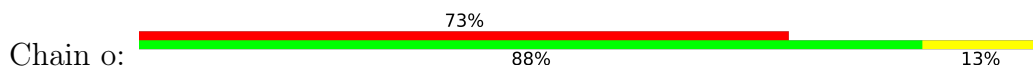




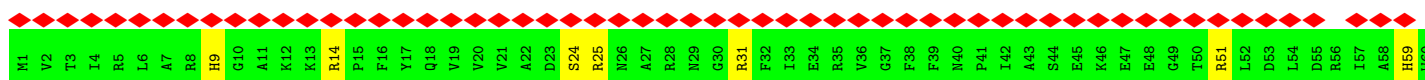
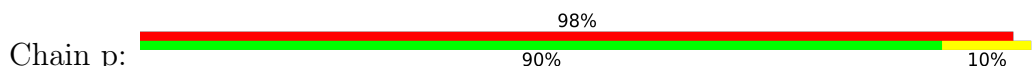
• Molecule 45: 30S ribosomal protein S14



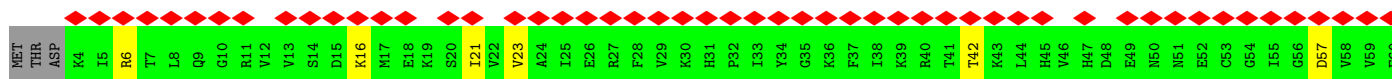
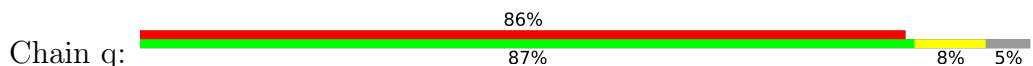
• Molecule 46: 30S ribosomal protein S15



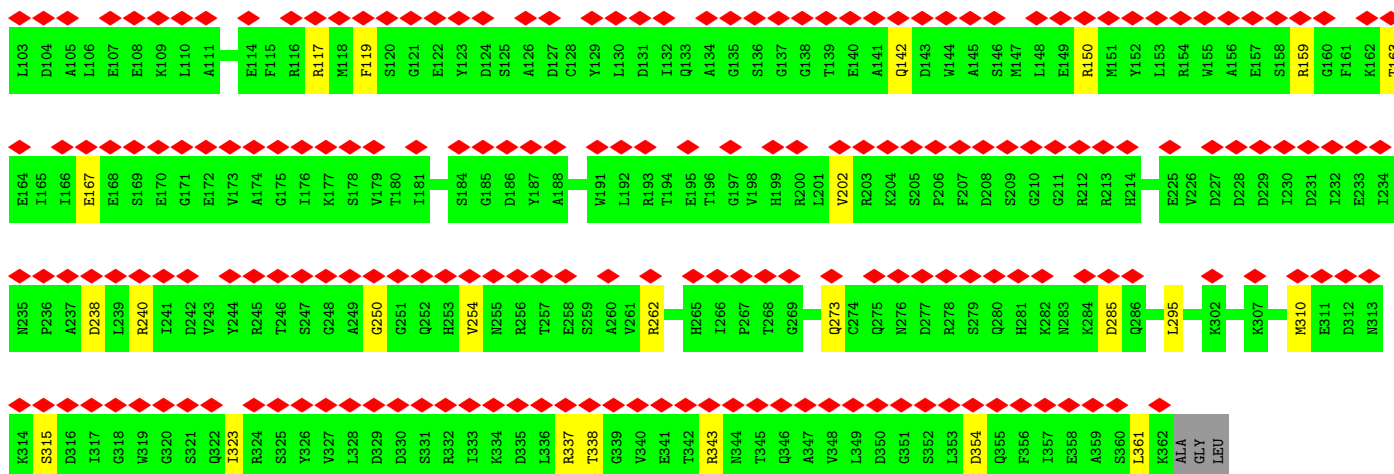
• Molecule 47: 30S ribosomal protein S16



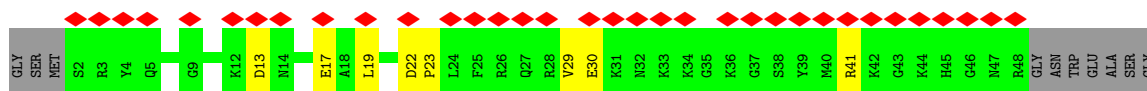
• Molecule 48: 30S ribosomal protein S17



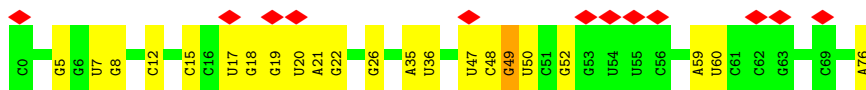
• Molecule 49: 30S ribosomal protein S18



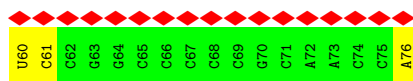
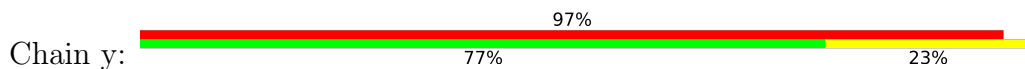
• Molecule 54: Alternative ribosome-rescue factor A



• Molecule 55: P-site or E-site fMet-tRNA(fMet)



• Molecule 55: P-site or E-site fMet-tRNA(fMet)



• Molecule 56: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	155440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	83822	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.118	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	458.112, 458.112, 458.112	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.193, 1.193, 1.193	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.23	0/69434	0.65	2/108325 (0.0%)
2	B	0.23	0/2828	0.65	0/4410
3	C	0.36	0/2121	0.65	0/2852
4	D	0.38	0/1586	0.61	0/2134
5	E	0.36	0/1571	0.66	0/2113
6	F	0.41	0/1434	0.65	0/1926
7	G	0.41	0/1343	0.64	0/1816
8	H	0.38	0/1122	0.63	0/1515
9	J	0.40	0/1046	0.61	0/1410
10	K	0.37	0/1152	0.65	0/1551
11	L	0.35	0/955	0.62	0/1279
12	M	0.37	0/1062	0.64	0/1413
13	N	0.39	0/1093	0.66	0/1460
14	O	0.42	0/973	0.74	0/1301
15	P	0.36	0/902	0.67	0/1209
16	Q	0.37	0/929	0.64	0/1242
17	R	0.41	0/960	0.70	0/1278
18	S	0.39	0/829	0.62	0/1107
19	T	0.34	0/864	0.69	0/1156
20	U	0.36	0/744	0.67	0/994
21	V	0.40	0/787	0.61	0/1051
22	W	0.38	0/766	0.61	0/1025
23	X	0.38	0/595	0.62	0/787
24	Y	0.38	0/635	0.67	0/848
25	Z	0.33	0/502	0.69	1/667 (0.1%)
26	0	0.36	0/453	0.68	1/605 (0.2%)
27	1	0.36	0/450	0.64	0/599
28	2	0.40	0/416	0.57	0/554
29	3	0.41	0/380	0.73	0/498
30	4	0.36	0/513	0.67	0/676
31	5	0.33	0/303	0.62	0/397
32	a	0.23	0/36593	0.66	1/57081 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.40	0/1784	0.62	0/2403
34	c	0.38	0/1651	0.66	0/2225
35	d	0.38	0/1655	0.68	0/2216
36	e	0.37	0/1169	0.65	0/1573
37	f	0.40	0/835	0.62	0/1128
38	g	0.38	0/1195	0.69	0/1602
39	h	0.36	0/989	0.65	0/1326
40	i	0.39	0/1034	0.70	0/1375
41	j	0.37	0/796	0.70	0/1077
42	k	0.38	0/893	0.60	0/1205
43	l	0.35	0/969	0.66	0/1300
44	m	0.62	2/892 (0.2%)	0.84	1/1193 (0.1%)
45	n	0.38	0/817	0.69	0/1088
46	o	0.37	0/722	0.68	0/964
47	p	0.39	0/659	0.64	0/884
48	q	0.38	0/657	0.66	0/881
49	r	0.40	0/548	0.63	0/736
50	s	0.46	1/675 (0.1%)	0.69	1/908 (0.1%)
51	t	0.37	0/676	0.67	0/895
52	u	0.43	0/472	0.73	0/627
53	v	0.38	0/2865	0.65	0/3858
54	w	0.35	0/394	0.63	0/519
55	x	0.24	0/1832	0.68	1/2855 (0.0%)
55	y	0.23	0/1832	0.65	0/2855
56	z	0.21	0/147	0.62	0/227
All	All	0.29	3/161499 (0.0%)	0.66	8/241199 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	m	90	ARG	CZ-NH1	13.28	1.50	1.33
44	m	90	ARG	CD-NE	5.57	1.55	1.46
50	s	55	ARG	CZ-NH1	5.15	1.39	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	m	90	ARG	NE-CZ-NH2	-14.43	113.09	120.30
50	s	55	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	2193	G	C2'-C3'-O3'	6.96	124.83	113.70
55	x	49	G	C2'-C3'-O3'	6.73	124.47	113.70
32	a	1517	G	C2'-C3'-O3'	6.38	123.91	113.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/273 (98%)	246 (91%)	20 (7%)	3 (1%)	14	52
4	D	207/209 (99%)	193 (93%)	13 (6%)	1 (0%)	29	68
5	E	199/201 (99%)	183 (92%)	14 (7%)	2 (1%)	15	54
6	F	175/179 (98%)	155 (89%)	16 (9%)	4 (2%)	6	36
7	G	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
8	H	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	11	46
9	J	139/142 (98%)	117 (84%)	16 (12%)	6 (4%)	2	22
10	K	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	22	61
11	L	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
12	M	142/144 (99%)	130 (92%)	11 (8%)	1 (1%)	22	61
13	N	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
14	O	118/127 (93%)	105 (89%)	12 (10%)	1 (1%)	19	58
15	P	114/117 (97%)	103 (90%)	10 (9%)	1 (1%)	17	56
16	Q	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
17	R	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
18	S	101/103 (98%)	90 (89%)	8 (8%)	3 (3%)	4	30
19	T	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	17	56
20	U	91/100 (91%)	83 (91%)	6 (7%)	2 (2%)	6	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	V	100/104 (96%)	82 (82%)	17 (17%)	1 (1%)	15	54
22	W	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
23	X	75/85 (88%)	68 (91%)	6 (8%)	1 (1%)	12	48
24	Y	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
25	Z	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	9	42
26	0	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	8	41
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	48/55 (87%)	44 (92%)	3 (6%)	1 (2%)	7	38
29	3	44/46 (96%)	44 (100%)	0	0	100	100
30	4	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	5	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
33	b	222/241 (92%)	207 (93%)	14 (6%)	1 (0%)	29	68
34	c	204/233 (88%)	192 (94%)	10 (5%)	2 (1%)	15	54
35	d	202/206 (98%)	192 (95%)	10 (5%)	0	100	100
36	e	155/167 (93%)	145 (94%)	8 (5%)	2 (1%)	12	48
37	f	98/135 (73%)	93 (95%)	4 (4%)	1 (1%)	15	54
38	g	149/179 (83%)	141 (95%)	8 (5%)	0	100	100
39	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
40	i	125/130 (96%)	112 (90%)	10 (8%)	3 (2%)	6	35
41	j	96/103 (93%)	87 (91%)	6 (6%)	3 (3%)	4	30
42	k	115/117 (98%)	103 (90%)	11 (10%)	1 (1%)	17	56
43	l	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	19	58
44	m	112/118 (95%)	105 (94%)	7 (6%)	0	100	100
45	n	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
46	o	86/88 (98%)	83 (96%)	2 (2%)	1 (1%)	13	50
47	p	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
48	q	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
49	r	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
50	s	80/82 (98%)	74 (92%)	5 (6%)	1 (1%)	12	48
51	t	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
52	u	54/71 (76%)	54 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	v	354/383 (92%)	334 (94%)	19 (5%)	1 (0%)	41	75
54	w	45/57 (79%)	39 (87%)	5 (11%)	1 (2%)	6	37
All	All	6056/6398 (95%)	5615 (93%)	390 (6%)	51 (1%)	24	58

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	241	GLY
5	E	64	GLY
18	S	82	HIS
6	F	174	ASP
9	J	20	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	216/218 (99%)	198 (92%)	18 (8%)	11	40
4	D	164/164 (100%)	153 (93%)	11 (7%)	16	48
5	E	165/165 (100%)	159 (96%)	6 (4%)	35	66
6	F	148/150 (99%)	136 (92%)	12 (8%)	11	41
7	G	137/138 (99%)	132 (96%)	5 (4%)	35	66
8	H	114/114 (100%)	109 (96%)	5 (4%)	28	62
9	J	109/110 (99%)	103 (94%)	6 (6%)	21	54
10	K	116/116 (100%)	114 (98%)	2 (2%)	60	82
11	L	104/104 (100%)	96 (92%)	8 (8%)	13	42
12	M	103/103 (100%)	96 (93%)	7 (7%)	16	48
13	N	109/109 (100%)	103 (94%)	6 (6%)	21	54
14	O	100/103 (97%)	95 (95%)	5 (5%)	24	58
15	P	86/87 (99%)	78 (91%)	8 (9%)	9	35
16	Q	99/100 (99%)	93 (94%)	6 (6%)	18	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	R	89/90 (99%)	81 (91%)	8 (9%)	9	37
18	S	84/84 (100%)	81 (96%)	3 (4%)	35	66
19	T	93/93 (100%)	92 (99%)	1 (1%)	73	88
20	U	80/84 (95%)	78 (98%)	2 (2%)	47	75
21	V	83/85 (98%)	78 (94%)	5 (6%)	19	52
22	W	78/78 (100%)	69 (88%)	9 (12%)	5	26
23	X	59/63 (94%)	55 (93%)	4 (7%)	16	48
24	Y	67/68 (98%)	60 (90%)	7 (10%)	7	31
25	Z	54/55 (98%)	53 (98%)	1 (2%)	57	80
26	0	48/49 (98%)	48 (100%)	0	100	100
27	1	47/48 (98%)	45 (96%)	2 (4%)	29	62
28	2	45/49 (92%)	44 (98%)	1 (2%)	52	78
29	3	38/38 (100%)	38 (100%)	0	100	100
30	4	51/52 (98%)	51 (100%)	0	100	100
31	5	34/34 (100%)	34 (100%)	0	100	100
33	b	186/199 (94%)	172 (92%)	14 (8%)	13	43
34	c	170/190 (90%)	153 (90%)	17 (10%)	7	32
35	d	171/173 (99%)	157 (92%)	14 (8%)	11	40
36	e	119/126 (94%)	107 (90%)	12 (10%)	7	32
37	f	87/116 (75%)	82 (94%)	5 (6%)	20	53
38	g	124/147 (84%)	116 (94%)	8 (6%)	17	50
39	h	104/104 (100%)	98 (94%)	6 (6%)	20	53
40	i	105/107 (98%)	95 (90%)	10 (10%)	8	34
41	j	86/90 (96%)	76 (88%)	10 (12%)	5	26
42	k	90/90 (100%)	88 (98%)	2 (2%)	52	78
43	l	103/103 (100%)	96 (93%)	7 (7%)	16	48
44	m	92/96 (96%)	85 (92%)	7 (8%)	13	43
45	n	83/83 (100%)	76 (92%)	7 (8%)	11	40
46	o	76/76 (100%)	66 (87%)	10 (13%)	4	21
47	p	65/65 (100%)	57 (88%)	8 (12%)	4	23
48	q	74/78 (95%)	67 (90%)	7 (10%)	8	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	r	57/66 (86%)	53 (93%)	4 (7%)	15	46
50	s	72/72 (100%)	65 (90%)	7 (10%)	8	33
51	t	65/65 (100%)	61 (94%)	4 (6%)	18	51
52	u	48/61 (79%)	46 (96%)	2 (4%)	30	63
53	v	304/324 (94%)	274 (90%)	30 (10%)	8	33
54	w	40/46 (87%)	33 (82%)	7 (18%)	2	10
All	All	5041/5228 (96%)	4695 (93%)	346 (7%)	19	47

5 of 346 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	i	124	ARG
48	q	16	LYS
41	j	31	ARG
45	n	20	TYR
50	s	55	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
36	e	135	ASN
43	l	6	GLN
36	e	146	ASN
38	g	86	GLN
47	p	63	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2903/2904 (99%)	855 (29%)	82 (2%)
2	B	117/118 (99%)	35 (29%)	1 (0%)
32	a	1529/1533 (99%)	490 (32%)	0
55	x	76/77 (98%)	22 (28%)	0
55	y	76/77 (98%)	18 (23%)	0
56	z	5/18 (27%)	1 (20%)	0
All	All	4706/4727 (99%)	1421 (30%)	83 (1%)

5 of 1421 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	13	A
1	A	14	A
1	A	23	G
1	A	27	G

5 of 83 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1937	A
1	A	2517	C
1	A	2074	U
1	A	2286	G
1	A	2602	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	5MC	a	1407	32	18,22,23	0.92	1 (5%)	26,32,35	1.32	4 (15%)
32	5MC	a	967	32	18,22,23	1.05	1 (5%)	26,32,35	1.33	6 (23%)
1	PSU	A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	1.87	4 (18%)
1	PSU	A	2457	1	18,21,22	1.45	3 (16%)	22,30,33	1.99	4 (18%)
53	MEQ	v	252	53	8,9,10	0.46	0	5,10,12	0.44	0
1	5MU	A	1939	1	19,22,23	1.48	5 (26%)	28,32,35	2.06	7 (25%)
1	OMG	A	2251	55,1	18,26,27	1.08	2 (11%)	19,38,41	1.10	2 (10%)
1	PSU	A	746	1,57	18,21,22	1.37	2 (11%)	22,30,33	1.95	3 (13%)
1	PSU	A	2504	1	18,21,22	1.31	2 (11%)	22,30,33	2.14	6 (27%)
32	MA6	a	1519	32	19,26,27	1.17	2 (10%)	18,38,41	1.96	7 (38%)
32	2MG	a	966	32	18,26,27	0.97	0	16,38,41	1.41	2 (12%)
1	PSU	A	955	1	18,21,22	1.40	3 (16%)	22,30,33	1.90	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	2580	1	18,21,22	1.44	3 (16%)	22,30,33	2.12	5 (22%)
32	PSU	a	516	32	18,21,22	1.39	3 (16%)	22,30,33	1.94	5 (22%)
32	2MG	a	1516	32	18,26,27	0.95	1 (5%)	16,38,41	1.12	2 (12%)
32	2MG	a	1207	32	18,26,27	0.97	0	16,38,41	1.20	3 (18%)
1	5MC	A	1962	1	18,22,23	1.00	1 (5%)	26,32,35	1.39	4 (15%)
1	PSU	A	1917	1	18,21,22	1.36	3 (16%)	22,30,33	1.93	5 (22%)
1	OMU	A	2552	1	19,22,23	1.20	3 (15%)	26,31,34	1.76	6 (23%)
1	5MU	A	747	1	19,22,23	1.53	4 (21%)	28,32,35	2.13	11 (39%)
32	MA6	a	1518	32	19,26,27	1.14	2 (10%)	18,38,41	2.22	6 (33%)
1	OMC	A	2498	1,57	19,22,23	0.90	1 (5%)	26,31,34	1.24	3 (11%)
1	1MG	A	745	1	18,26,27	0.95	0	19,39,42	1.42	4 (21%)
1	2MG	A	2445	1	18,26,27	0.92	0	16,38,41	1.18	3 (18%)
32	UR3	a	1498	32	19,22,23	1.19	1 (5%)	26,32,35	1.71	5 (19%)
32	4OC	a	1402	32	20,23,24	0.84	0	26,32,35	1.24	4 (15%)
1	PSU	A	2605	1	18,21,22	1.42	2 (11%)	22,30,33	2.08	4 (18%)
1	2MG	A	1835	1	18,26,27	1.02	1 (5%)	16,38,41	1.16	2 (12%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	2/7/25/26	0/2/2/2
53	MEQ	v	252	53	-	1/8/9/11	-
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2
1	OMG	A	2251	55,1	-	0/5/27/28	0/3/3/3
1	PSU	A	746	1,57	-	3/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	0/7/25/26	0/2/2/2
32	MA6	a	1519	32	-	4/7/29/30	0/3/3/3
32	2MG	a	966	32	-	2/5/27/28	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
32	PSU	a	516	32	-	0/7/25/26	0/2/2/2
32	2MG	a	1516	32	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	2MG	a	1207	32	-	3/5/27/28	0/3/3/3
1	5MC	A	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	1	-	0/9/27/28	0/2/2/2
1	5MU	A	747	1	-	0/7/25/26	0/2/2/2
32	MA6	a	1518	32	-	4/7/29/30	0/3/3/3
1	OMC	A	2498	1,57	-	1/9/27/28	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
1	2MG	A	2445	1	-	2/5/27/28	0/3/3/3
32	UR3	a	1498	32	-	0/7/25/26	0/2/2/2
32	4OC	a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	2/5/27/28	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	516	PSU	C6-C5	4.31	1.40	1.35
1	A	955	PSU	C6-C5	4.18	1.40	1.35
1	A	2457	PSU	C6-C5	4.14	1.40	1.35
1	A	1911	PSU	C6-C5	3.95	1.39	1.35
1	A	746	PSU	C6-C5	3.89	1.39	1.35

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1518	MA6	N1-C6-N6	6.80	124.21	117.06
32	a	1498	UR3	C4-N3-C2	-6.43	118.51	124.56
1	A	2580	PSU	N1-C2-N3	6.31	122.28	115.13
1	A	2605	PSU	N1-C2-N3	6.18	122.14	115.13
1	A	2457	PSU	N1-C2-N3	6.12	122.06	115.13

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	746	PSU	O4'-C4'-C5'-O5'
1	A	2445	2MG	C3'-C4'-C5'-O5'
32	a	1402	4OC	O4'-C4'-C5'-O5'
32	a	1518	MA6	C5-C6-N6-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	v	252	MEQ	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 125 ligands modelled in this entry, 125 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

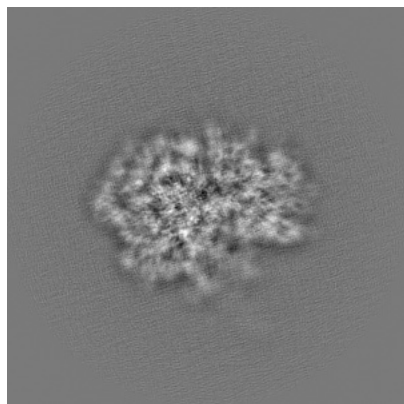
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8505. These allow visual inspection of the internal detail of the map and identification of artifacts.

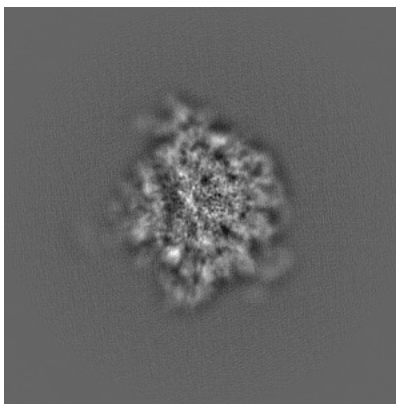
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

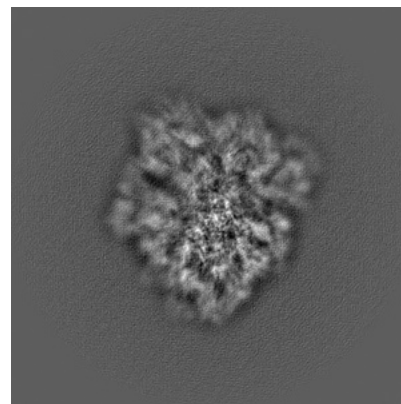
6.1.1 Primary map



X

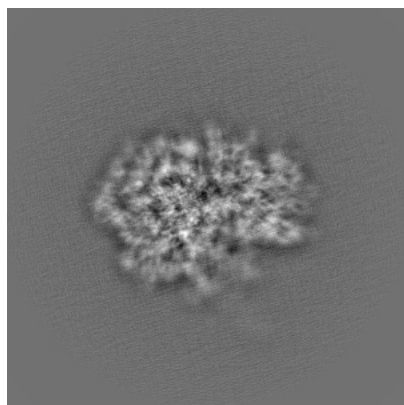


Y

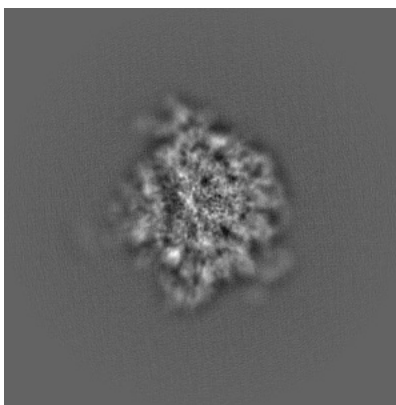


Z

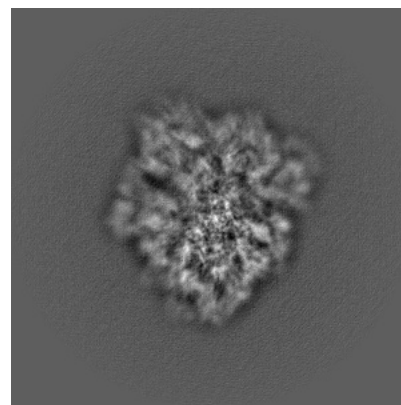
6.1.2 Raw map



X



Y

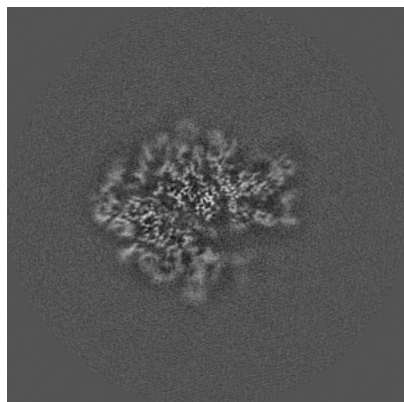


Z

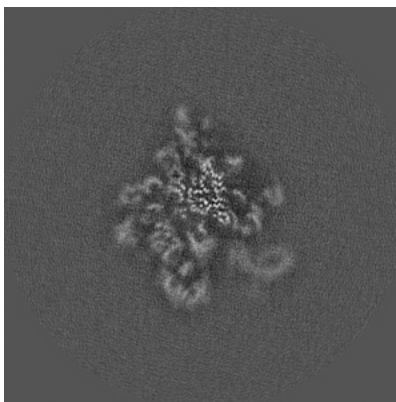
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

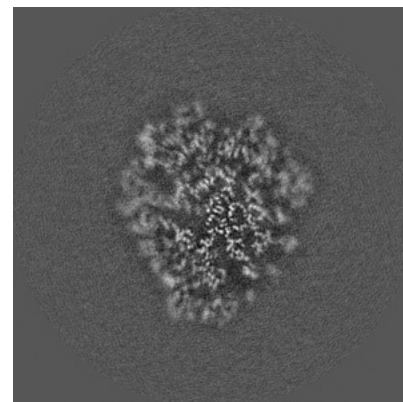
6.2.1 Primary map



X Index: 192

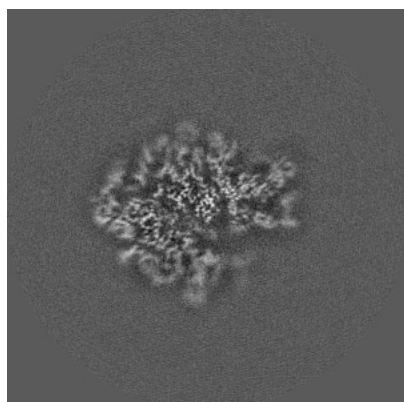


Y Index: 192

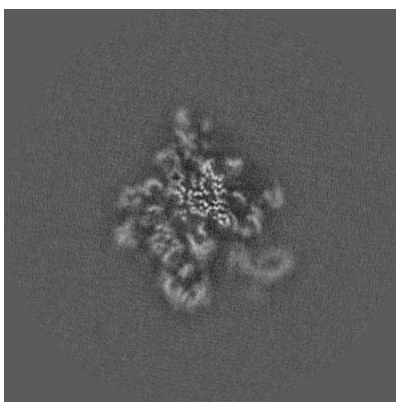


Z Index: 192

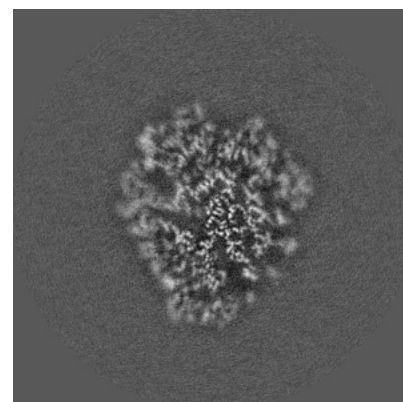
6.2.2 Raw map



X Index: 192



Y Index: 192

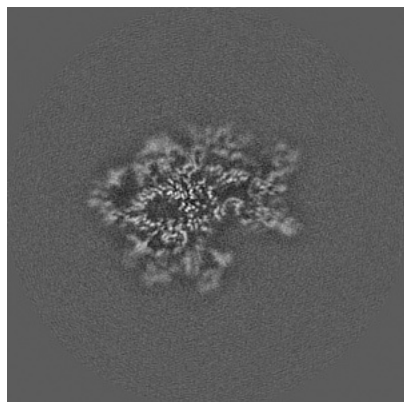


Z Index: 192

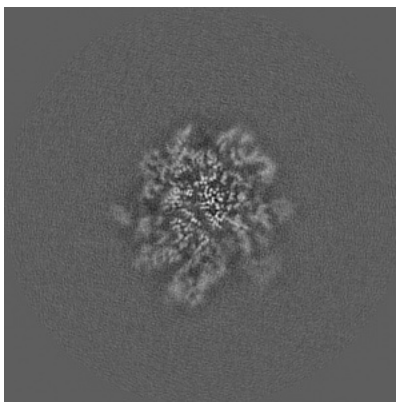
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

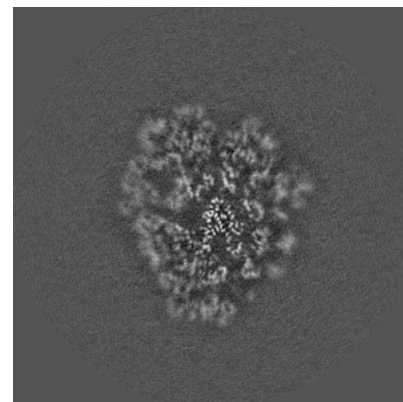
6.3.1 Primary map



X Index: 201

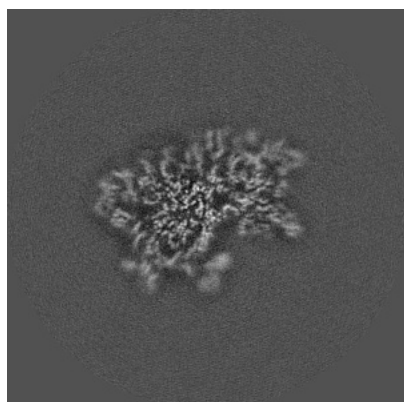


Y Index: 170

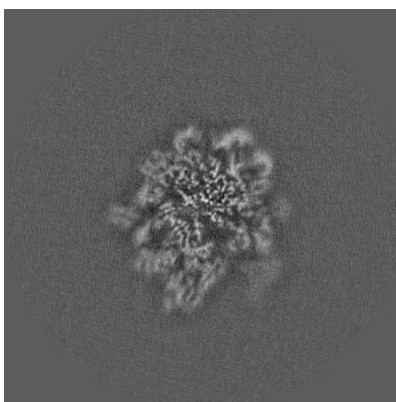


Z Index: 195

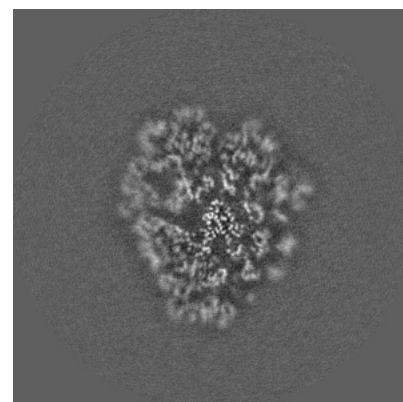
6.3.2 Raw map



X Index: 207



Y Index: 174

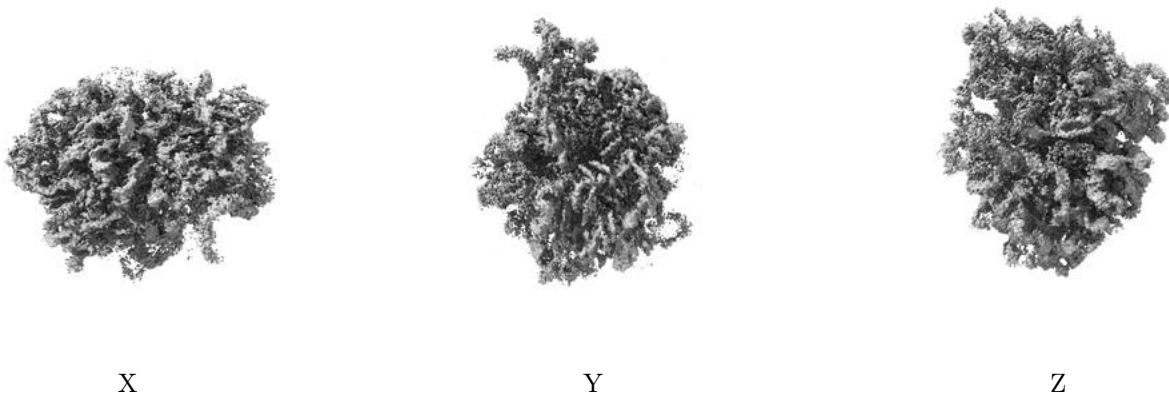


Z Index: 195

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

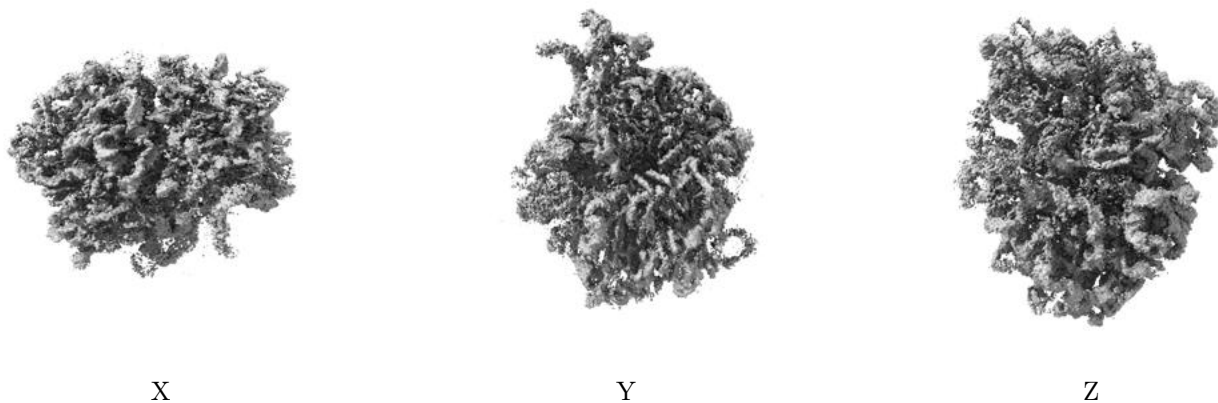
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

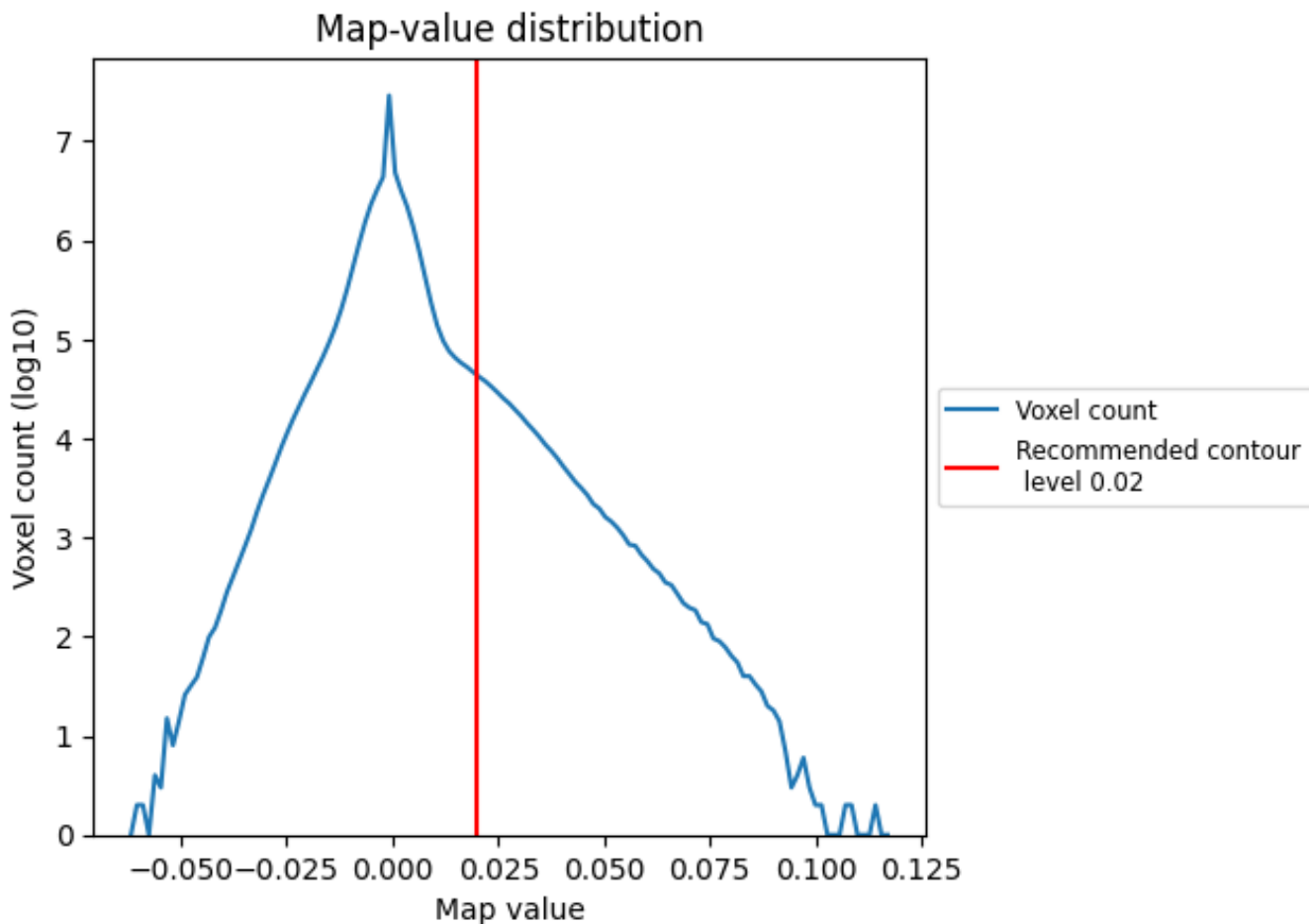
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

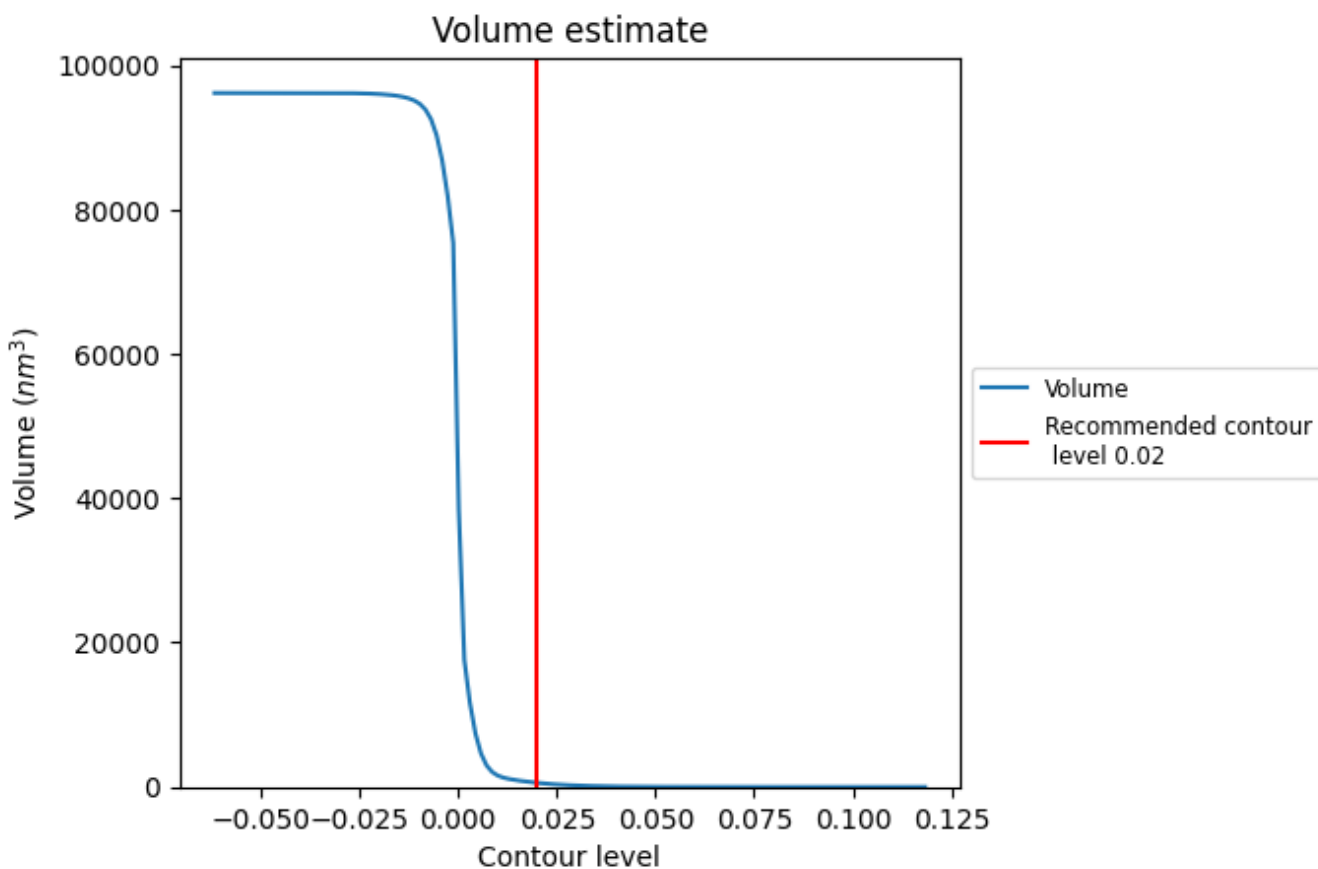
This section contains the results of statistical analysis of the map.

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.

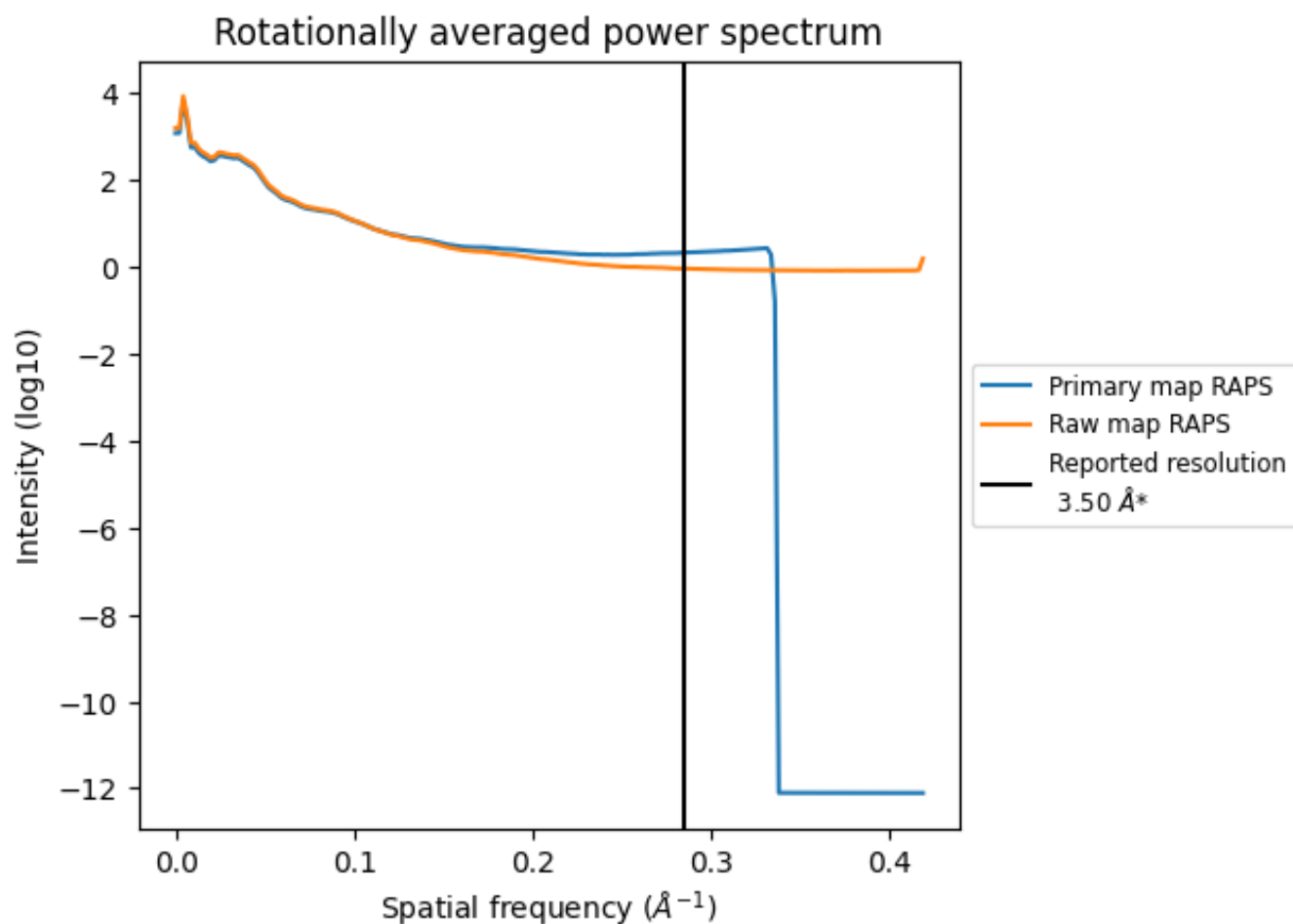
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 571 nm^3 ; this corresponds to an approximate mass of 516 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](#)

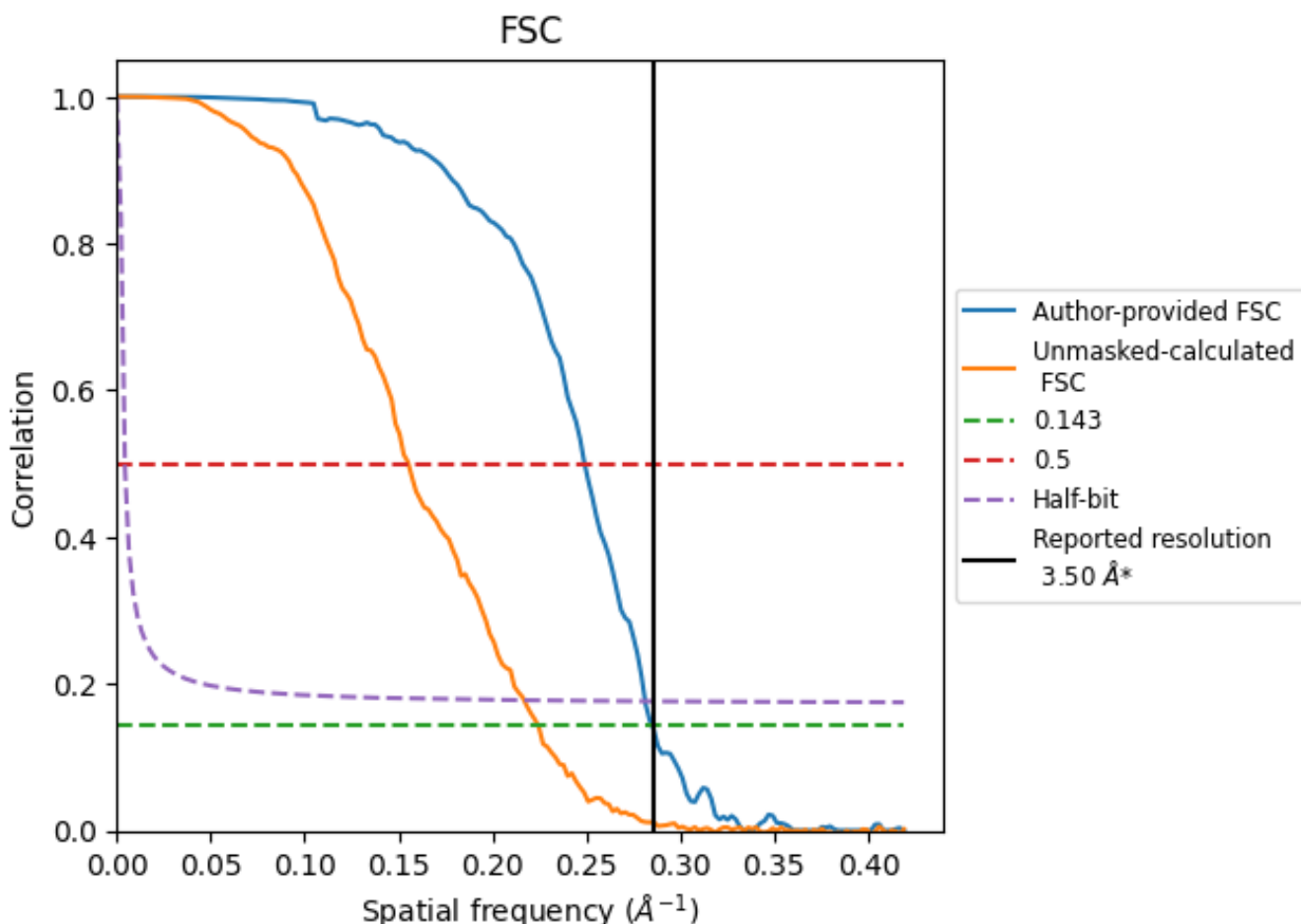


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

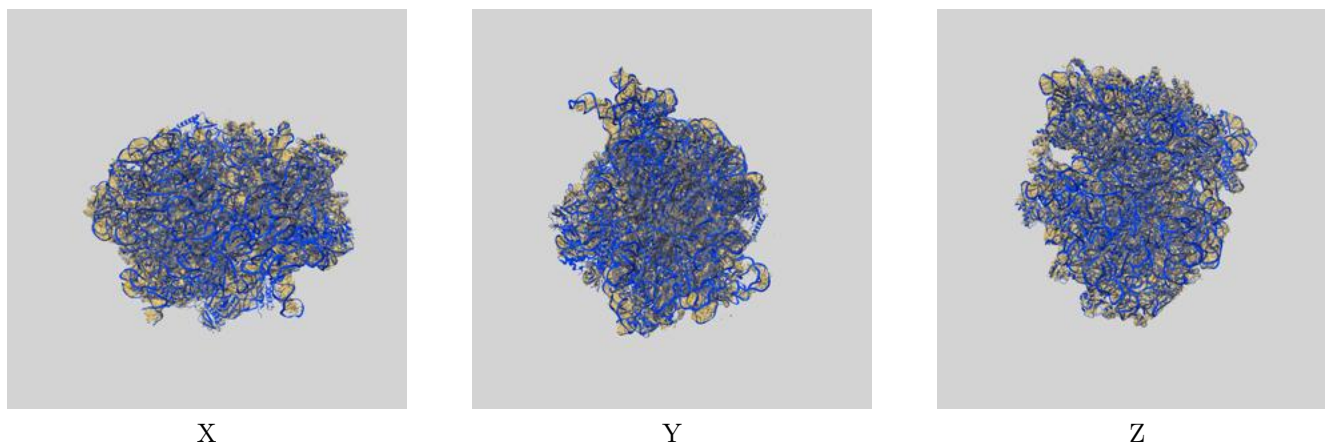
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	4.01	3.55
Unmasked-calculated*	4.46	6.44	4.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.46 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

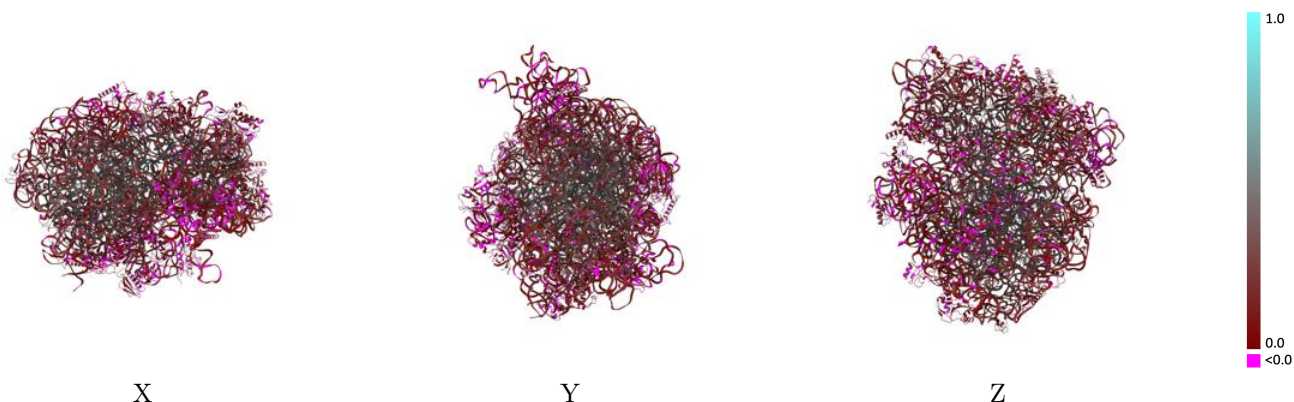
This section contains information regarding the fit between EMDB map EMD-8505 and PDB model 5U4I. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



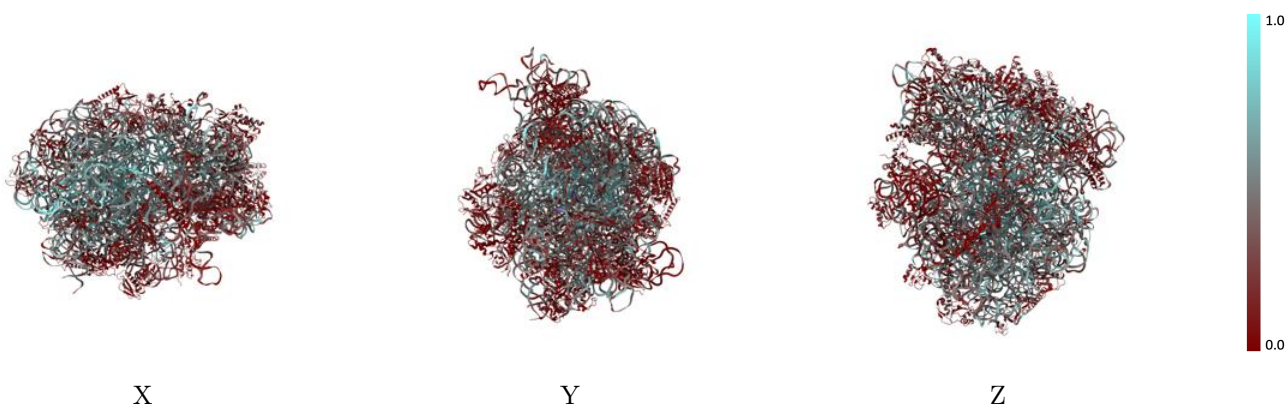
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



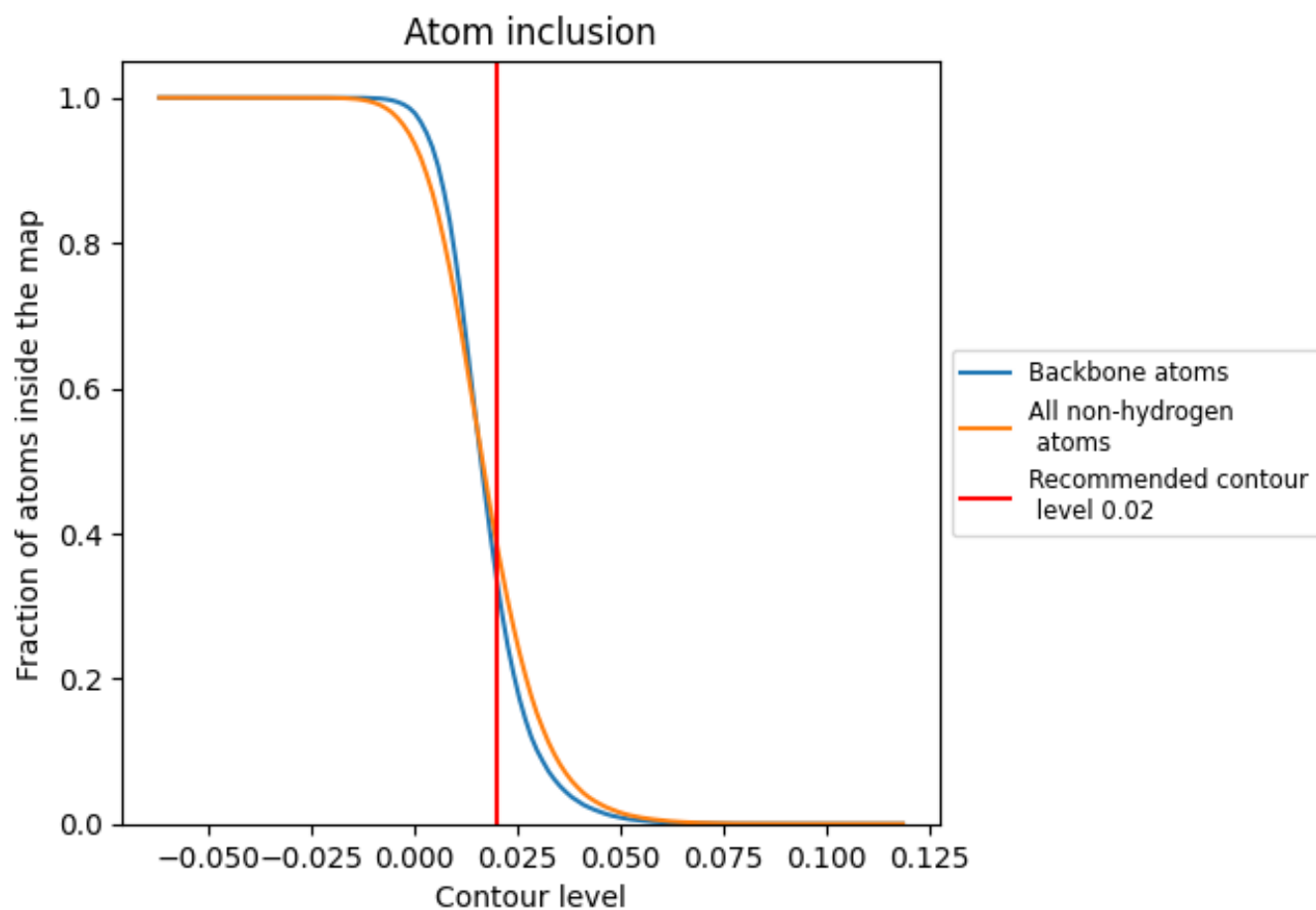
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 33% of all backbone atoms, 38% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3826	 0.2260
0	 0.1899	 0.1590
1	 0.2477	 0.2150
2	 0.0623	 0.0860
3	 0.3606	 0.3810
4	 0.0713	 0.2420
5	 0.0341	 0.1190
A	 0.5162	 0.2680
B	 0.3304	 0.1370
C	 0.2927	 0.2720
D	 0.1456	 0.1590
E	 0.2039	 0.1900
F	 0.1107	 0.1000
G	 0.0678	 0.0720
H	 0.0091	 0.0470
J	 0.0020	 0.0490
K	 0.0964	 0.1390
L	 0.2193	 0.2160
M	 0.1406	 0.1840
N	 0.1996	 0.1900
O	 0.1866	 0.2130
P	 0.0823	 0.0970
Q	 0.0935	 0.1020
R	 0.2159	 0.2310
S	 0.2146	 0.2020
T	 0.3696	 0.2930
U	 0.1870	 0.2110
V	 0.2086	 0.2040
W	 0.1057	 0.0790
X	 0.0857	 0.1640
Y	 0.0998	 0.1340
Z	 0.2270	 0.1710
a	 0.4513	 0.2410
b	 0.1411	 0.1220
c	 0.2433	 0.2010



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	 0.1000	 0.1590
e	 0.2734	 0.2490
f	 0.1721	 0.1020
g	 0.1766	 0.1410
h	 0.1698	 0.1550
i	 0.1205	 0.1520
j	 0.0986	 0.1540
k	 0.1512	 0.1510
l	 0.3094	 0.2900
m	 0.1469	 0.1640
n	 0.1434	 0.1670
o	 0.3029	 0.1620
p	 0.0447	 0.0090
q	 0.1234	 0.1480
r	 0.0695	 0.1120
s	 0.1137	 0.1500
t	 0.0336	 0.0500
u	 0.1937	 0.1490
v	 0.1827	 0.2170
w	 0.2819	 0.2930
x	 0.5738	 0.3170
y	 0.1067	 0.1170
z	 0.3282	 0.3360