



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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

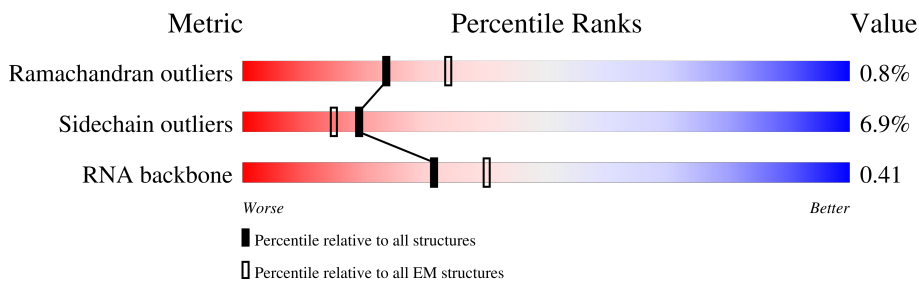
1 Overall quality at a glance i

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)
6	F	179	93% (0 outliers) 90% (1 outlier) 9% (2 outliers)
7	G	177	96% (0 outliers) 97% (1 outlier)
8	H	149	100% (0 outliers) 95% (1 outlier) 5% (2 outliers)

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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%

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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
			Total	C	N	O	S		
20	U	93	738	466	139	131	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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	S	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
33	b	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

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

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

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

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

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

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

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

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

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

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

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

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

- 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

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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	

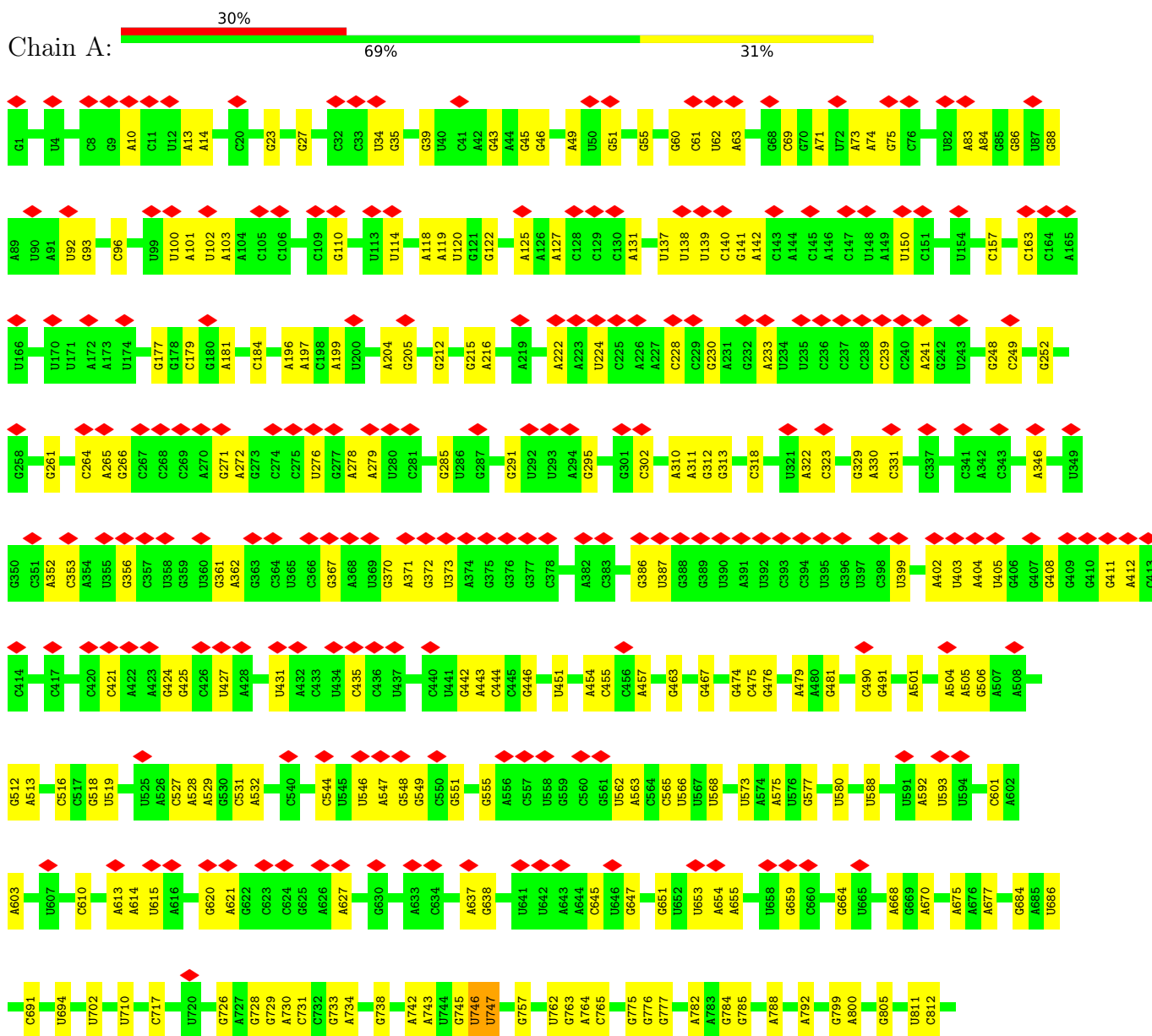
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

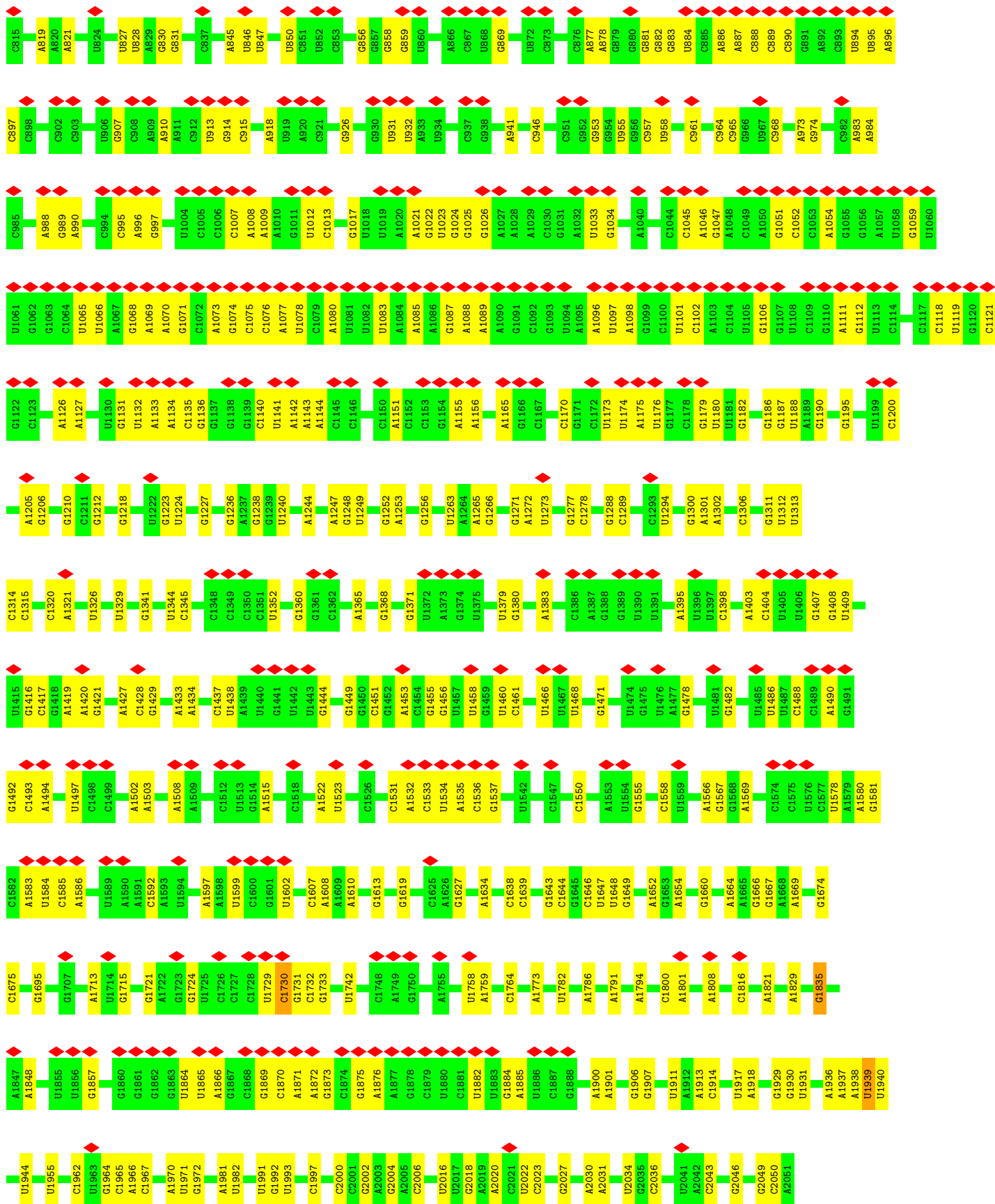
Mol	Chain	Residues	Atoms		AltConf
58	5	1	Total	Zn	0
			1	1	

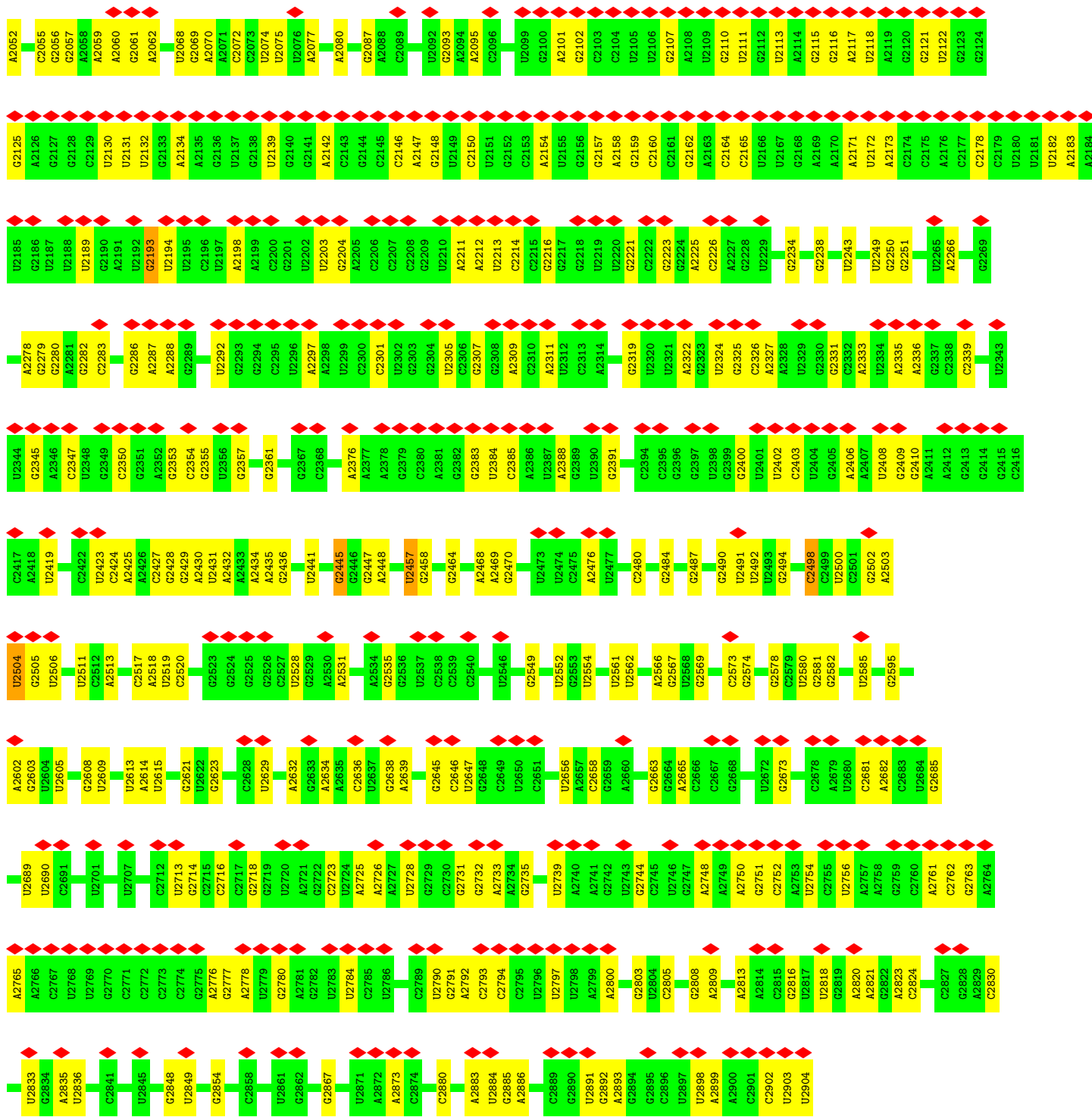
3 Residue-property plots

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.

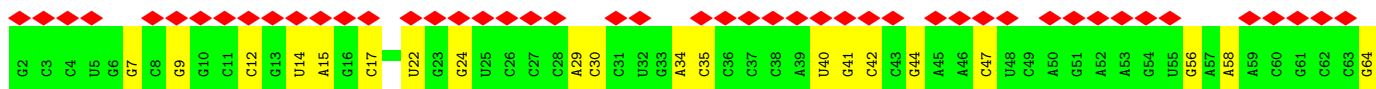
- Molecule 1: 23S rRNA

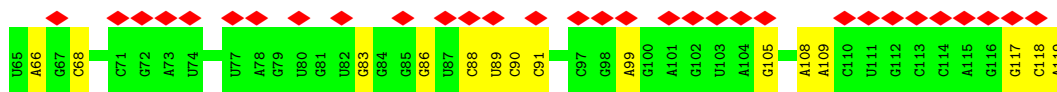




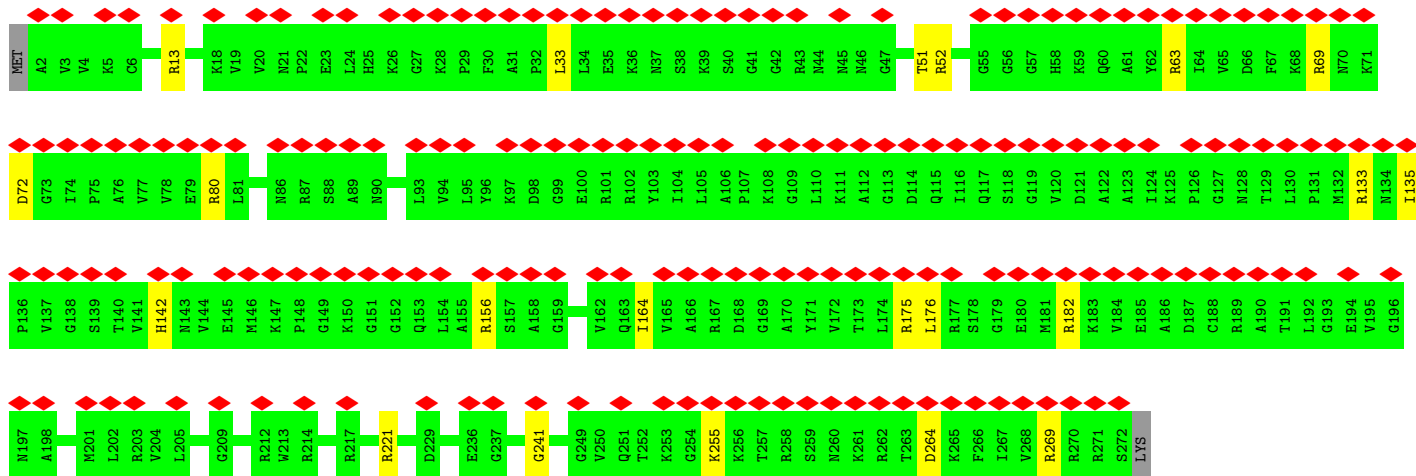
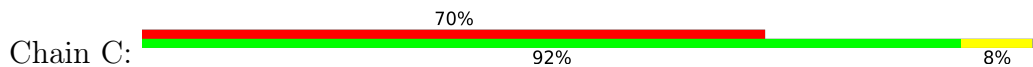


• Molecule 2: 5S rRNA

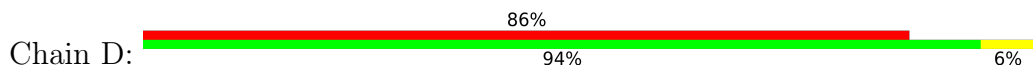




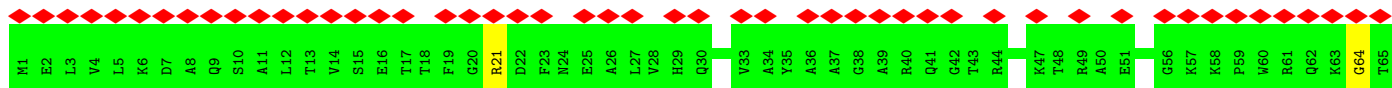
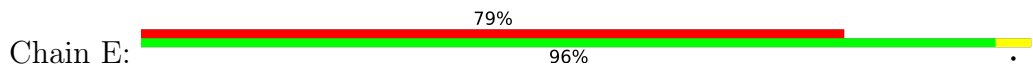
• Molecule 3: 50S ribosomal protein L2

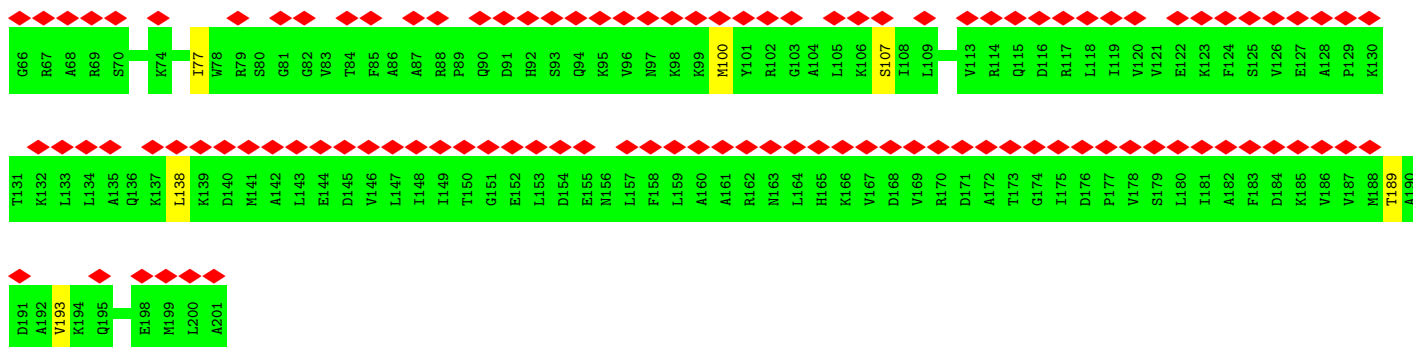


• Molecule 4: 50S ribosomal protein L3

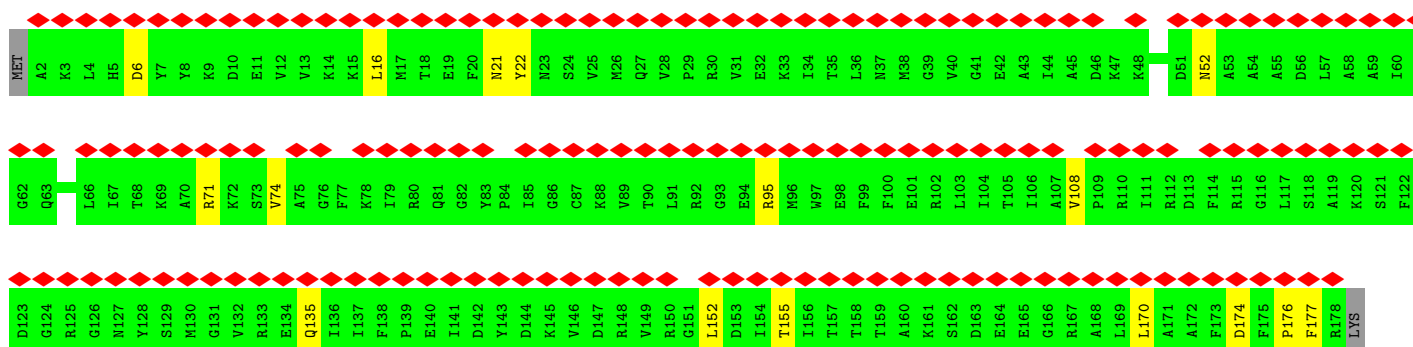
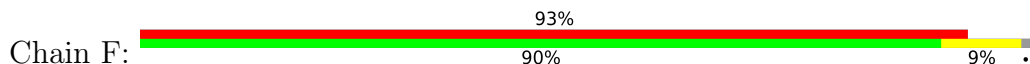


• Molecule 5: 50S ribosomal protein L4

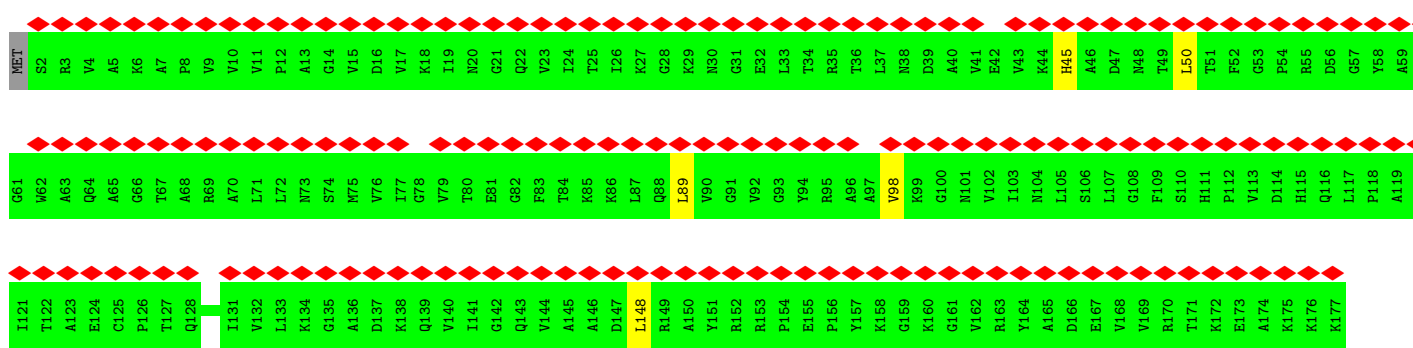




• Molecule 6: 50S ribosomal protein L5

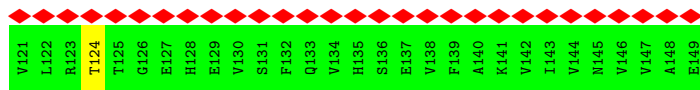


• Molecule 7: 50S ribosomal protein L6

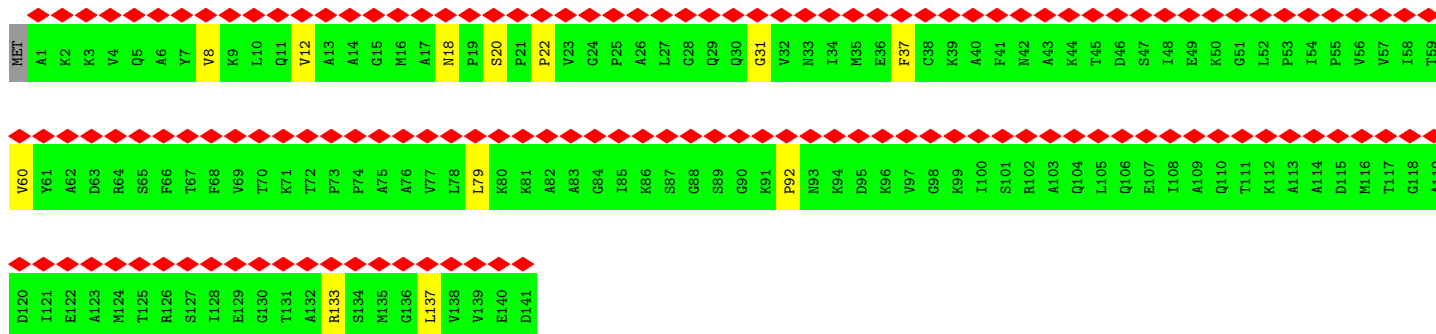
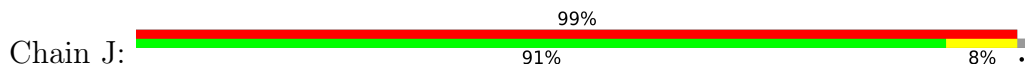


• Molecule 8: 50S ribosomal protein L9

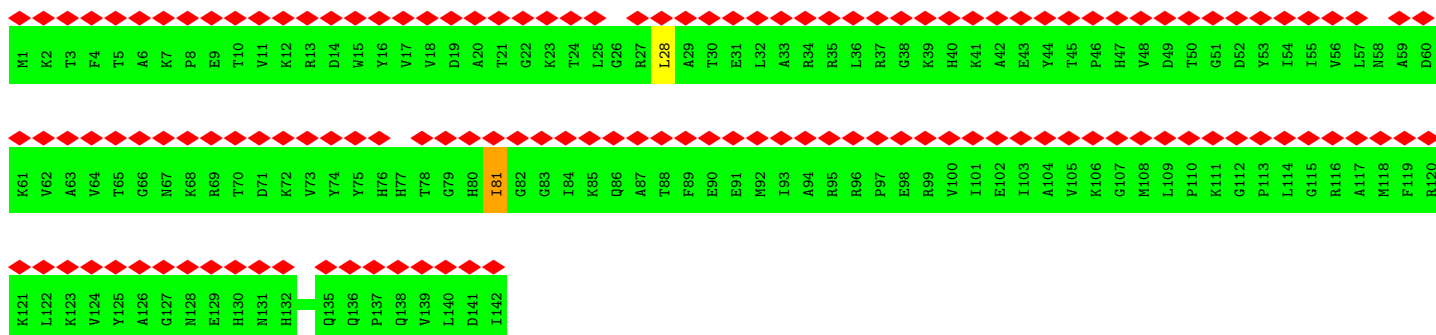




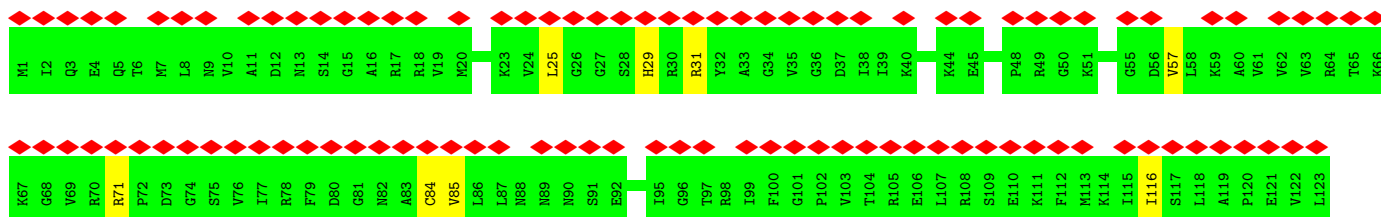
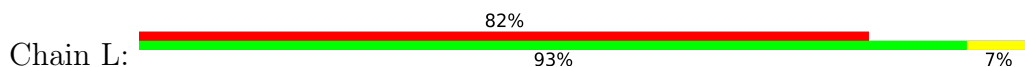
• Molecule 9: 50S ribosomal protein L11



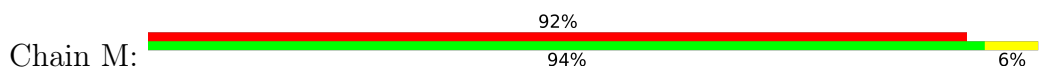
• Molecule 10: 50S ribosomal protein L13



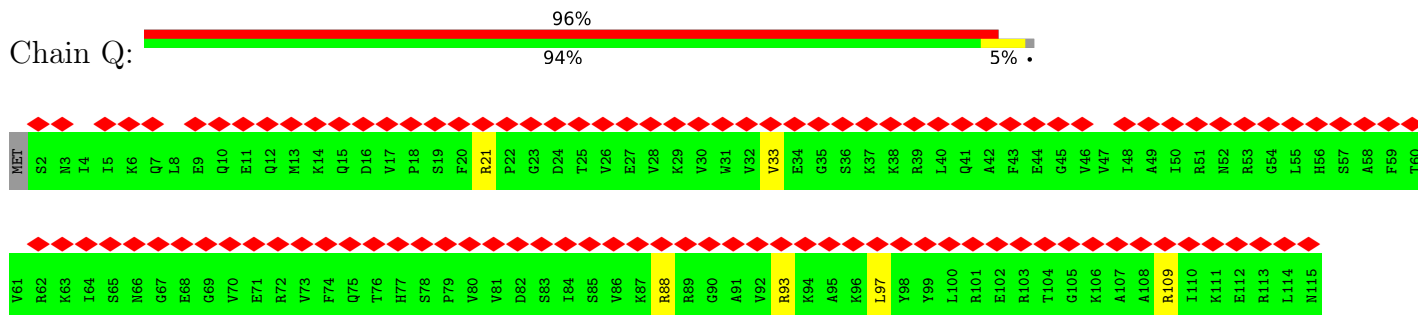
• Molecule 11: 50S ribosomal protein L14



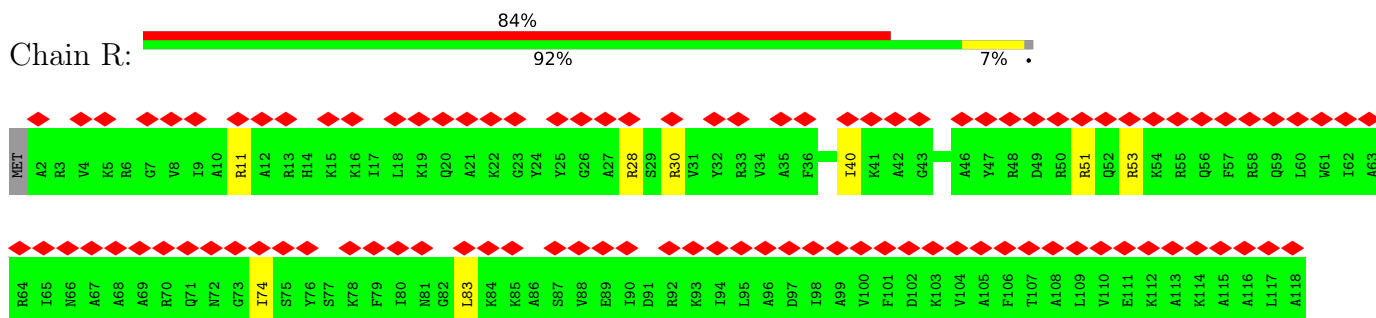
• Molecule 12: 50S ribosomal protein L15



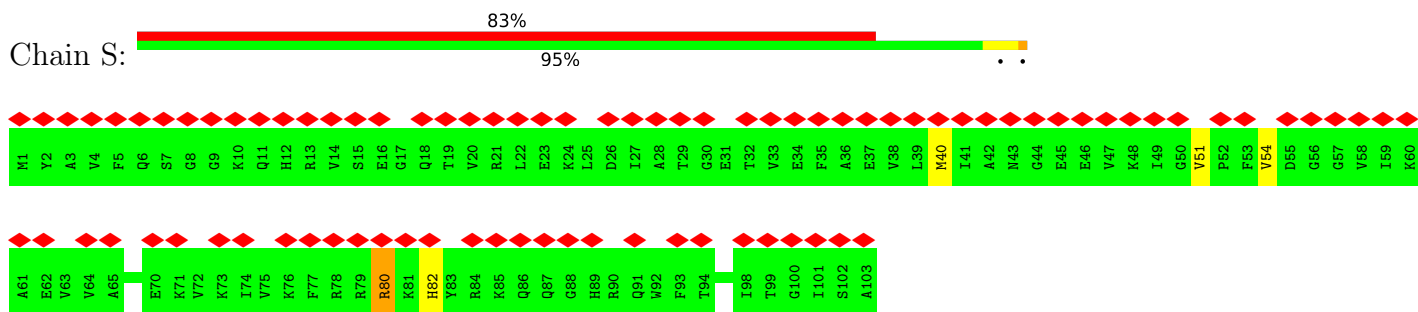
• Molecule 16: 50S ribosomal protein L19



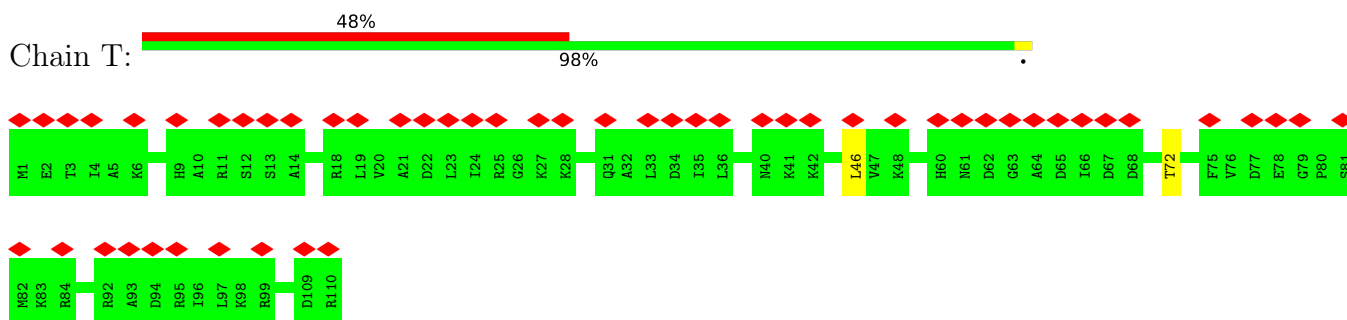
• Molecule 17: 50S ribosomal protein L20



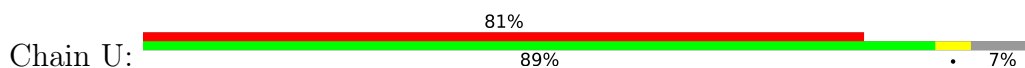
• Molecule 18: 50S ribosomal protein L21

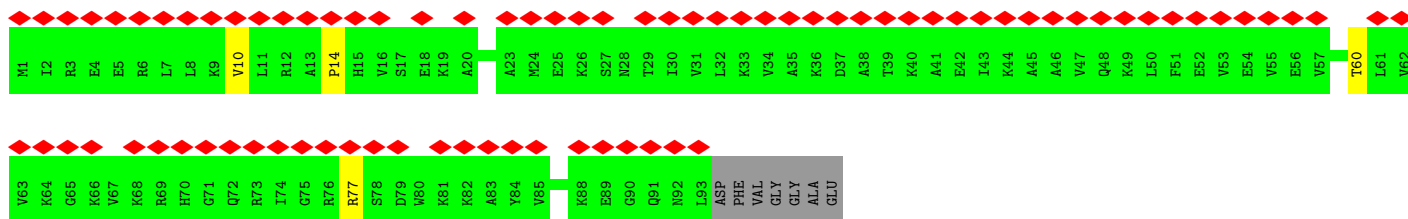


• Molecule 19: 50S ribosomal protein L22

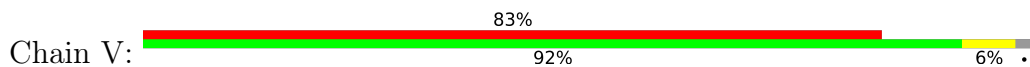


• Molecule 20: 50S ribosomal protein L23

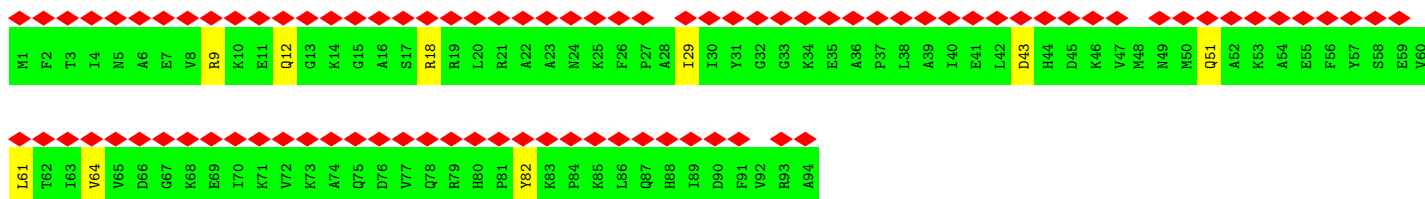




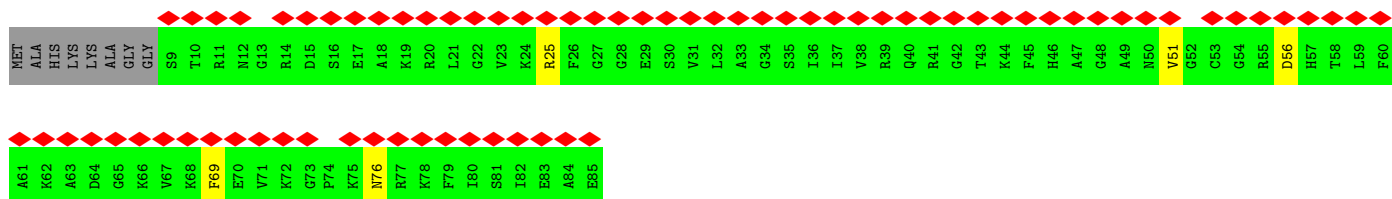
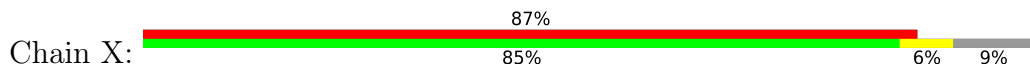
• Molecule 21: 50S ribosomal protein L24



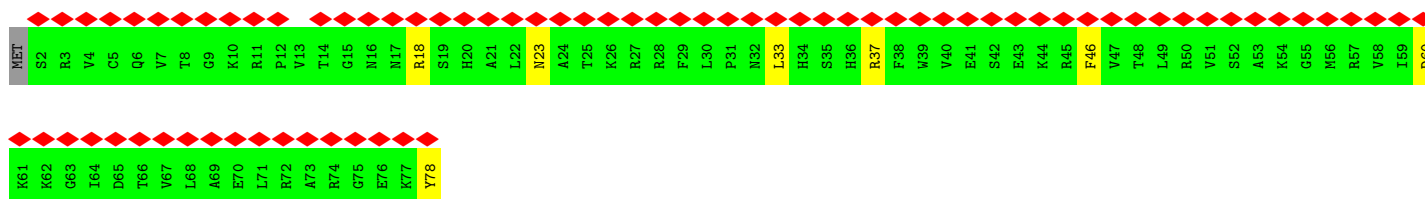
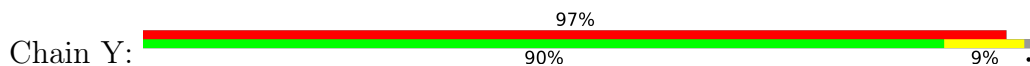
• Molecule 22: 50S ribosomal protein L25



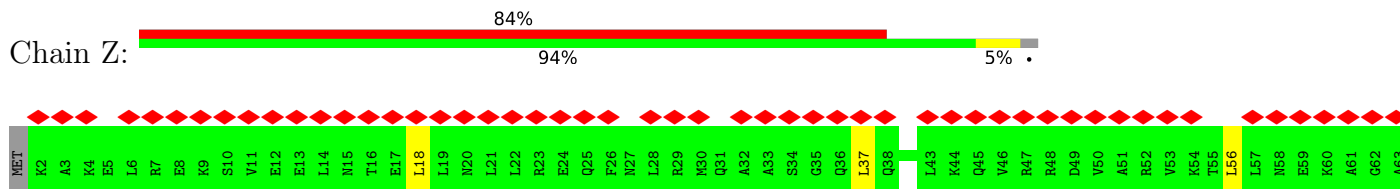
• Molecule 23: 50S ribosomal protein L27



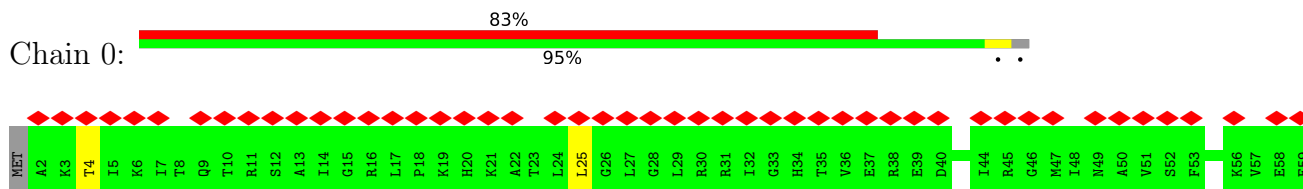
• Molecule 24: 50S ribosomal protein L28



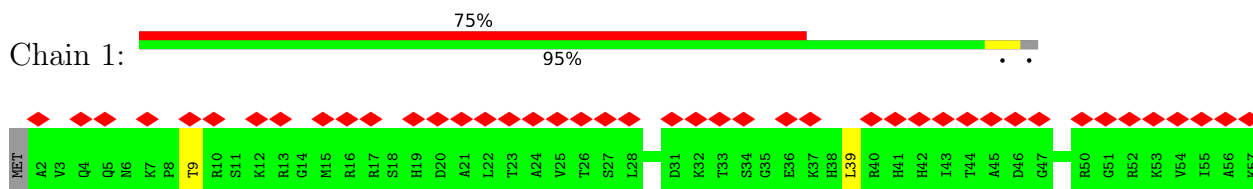
• Molecule 25: 50S ribosomal protein L29



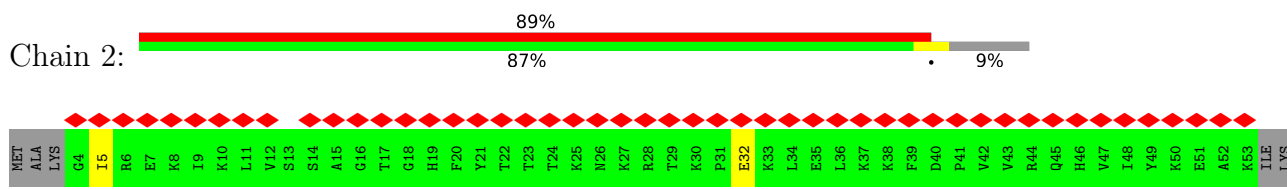
• Molecule 26: 50S ribosomal protein L30



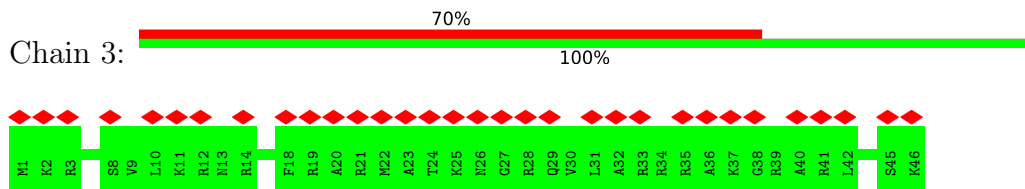
• Molecule 27: 50S ribosomal protein L32



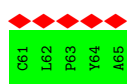
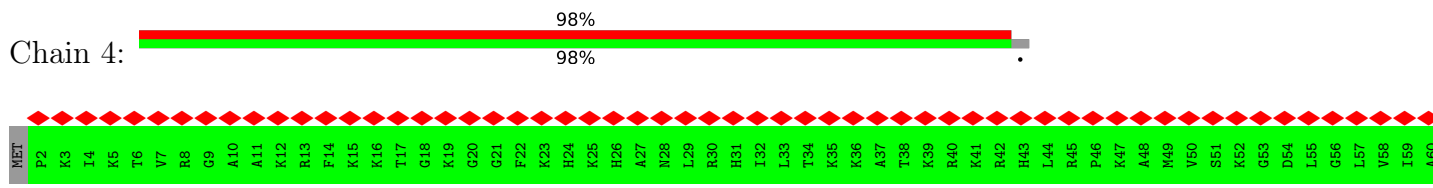
• Molecule 28: 50S ribosomal protein L33



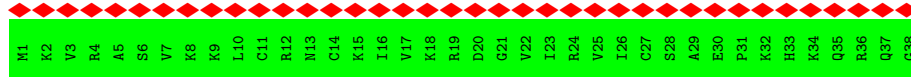
• Molecule 29: 50S ribosomal protein L34



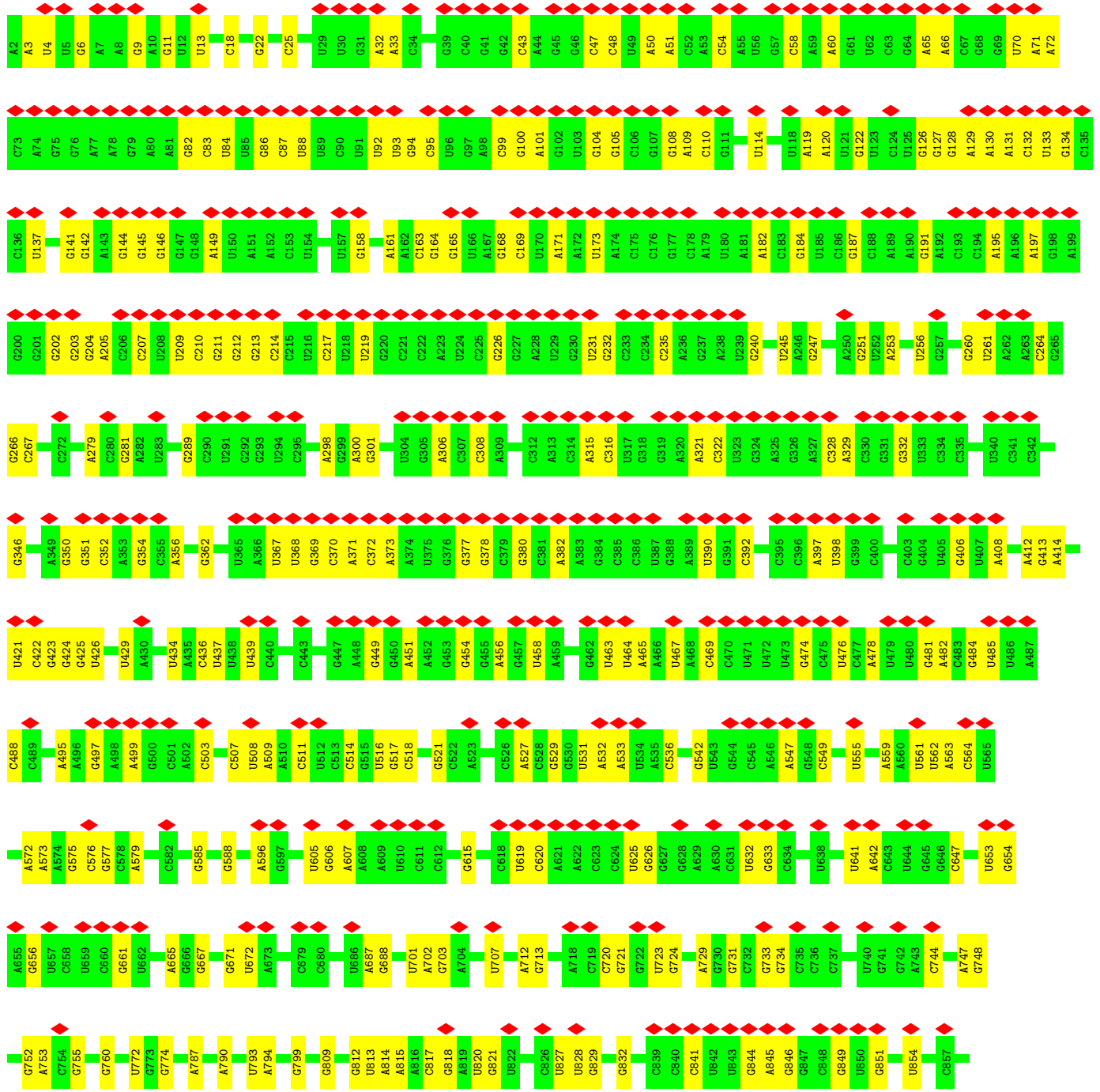
• Molecule 30: 50S ribosomal protein L35

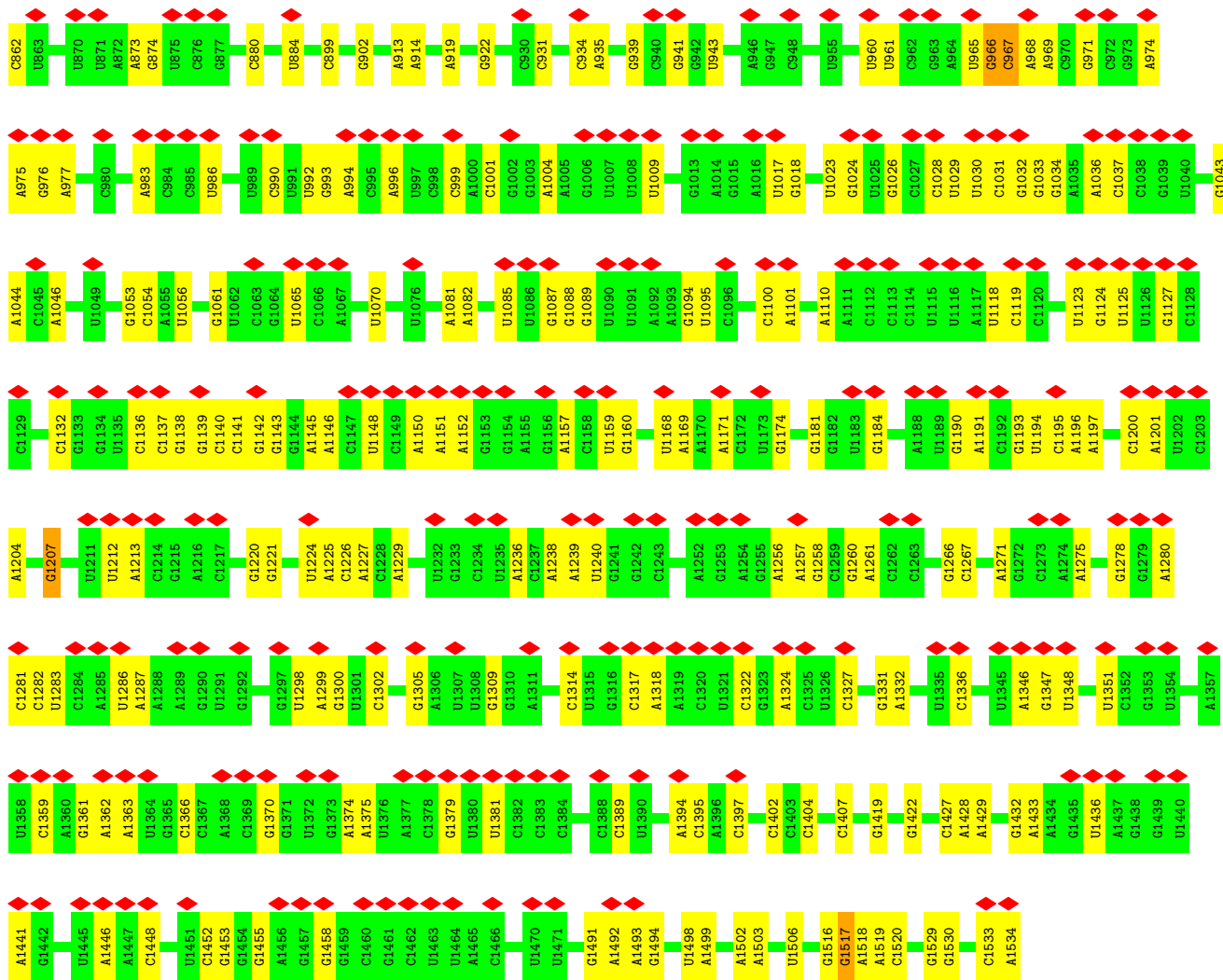


• Molecule 31: 50S ribosomal protein L36

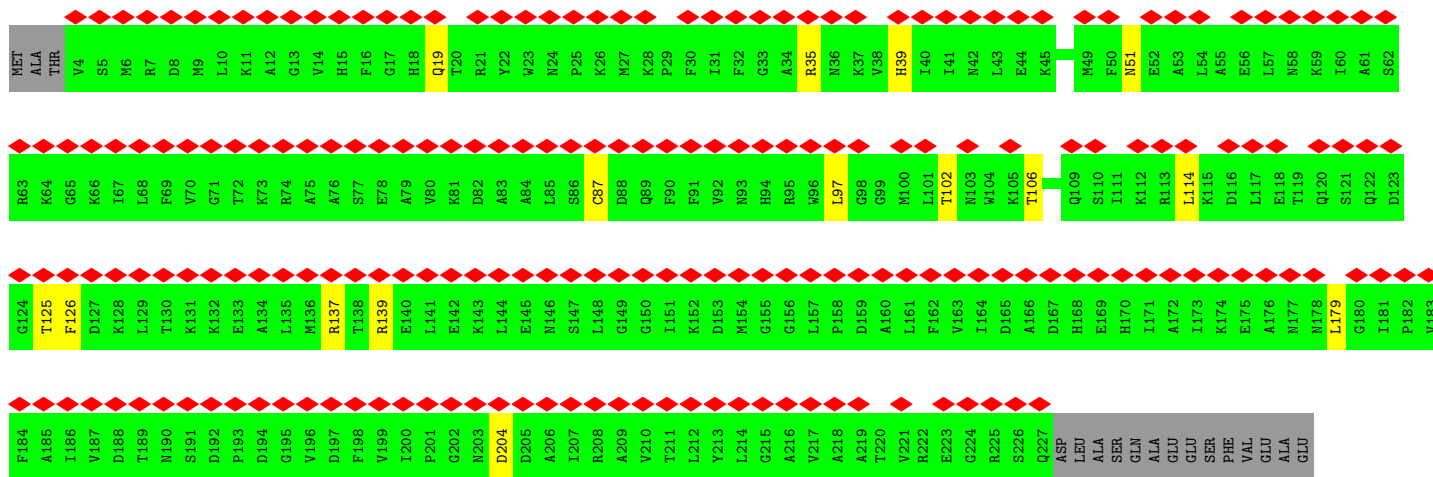
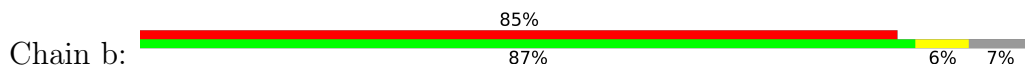


• Molecule 32: 16S rRNA

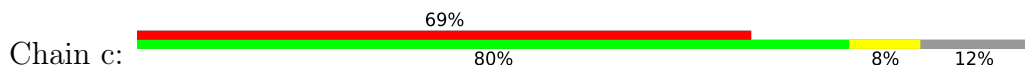




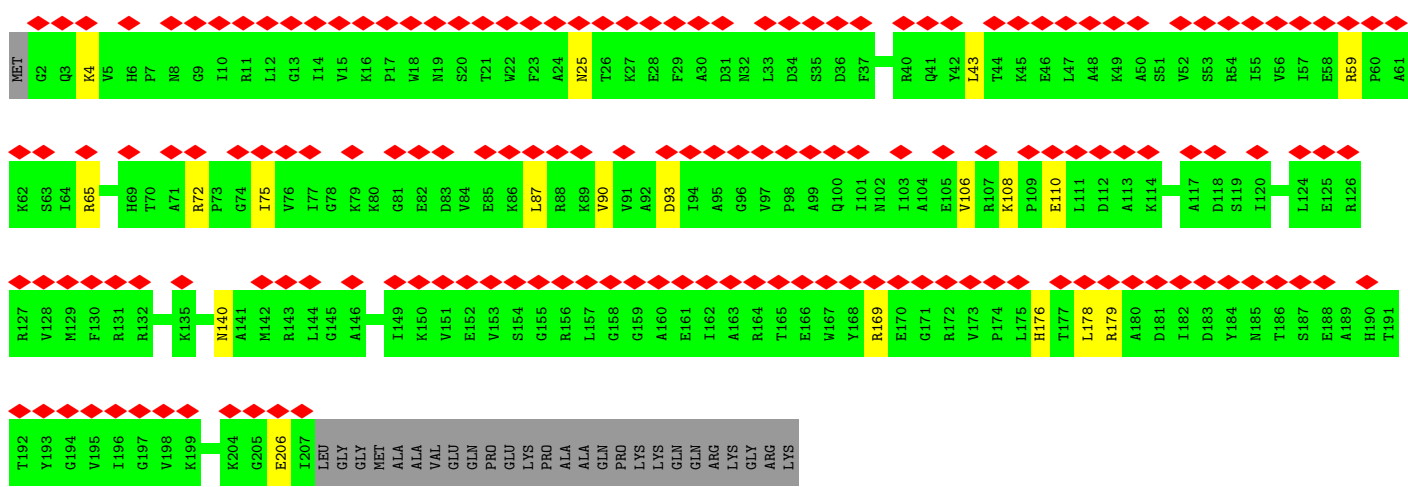
• Molecule 33: 30S ribosomal protein S2



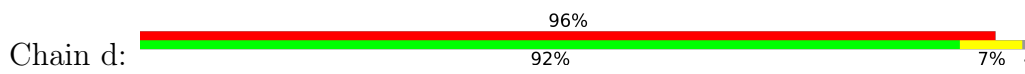
• Molecule 34: 30S ribosomal protein S3



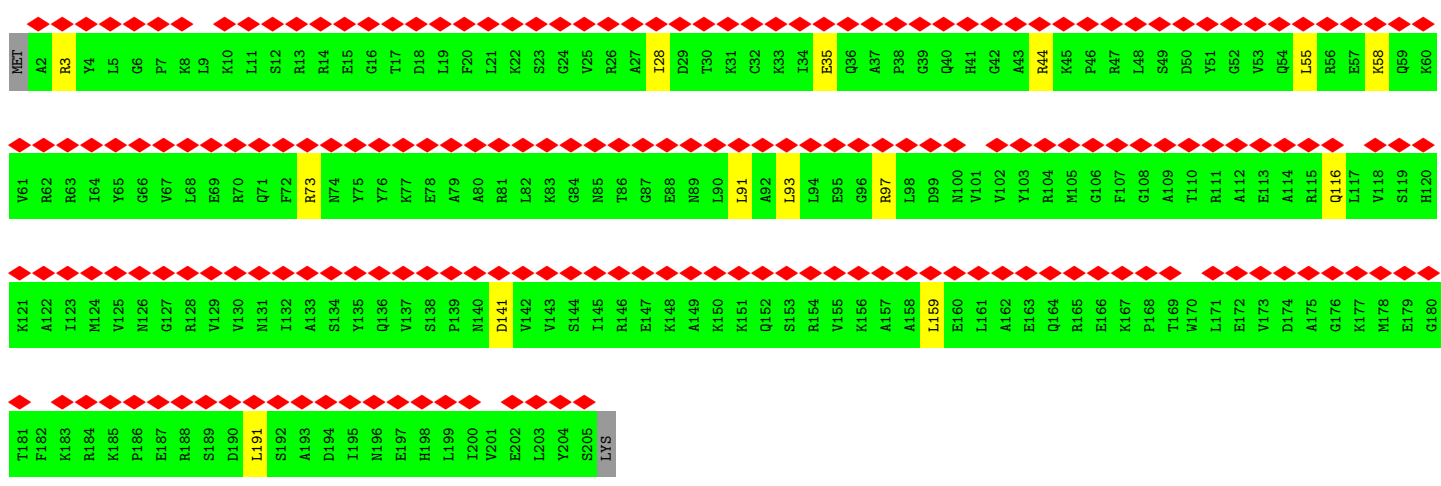
Chain c:



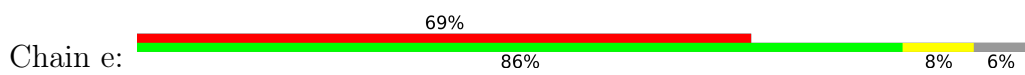
• Molecule 35: 30S ribosomal protein S4



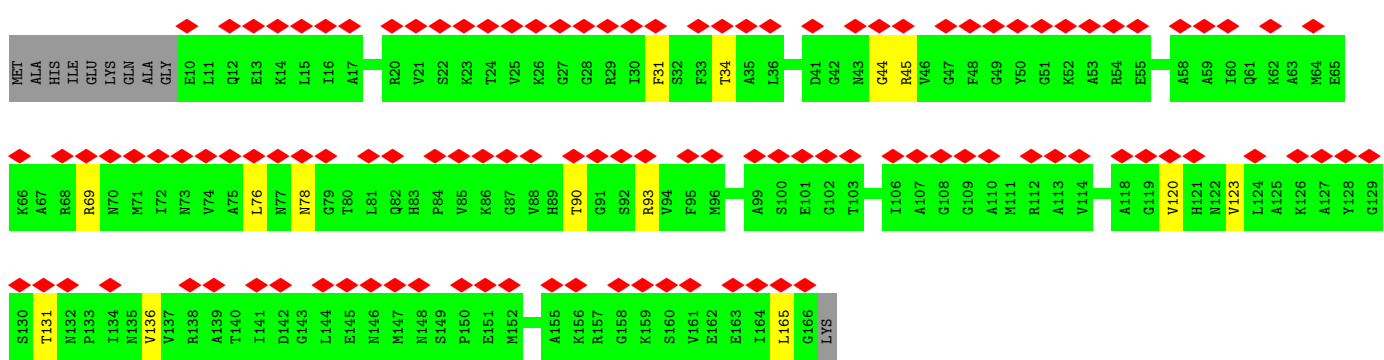
Chain d:



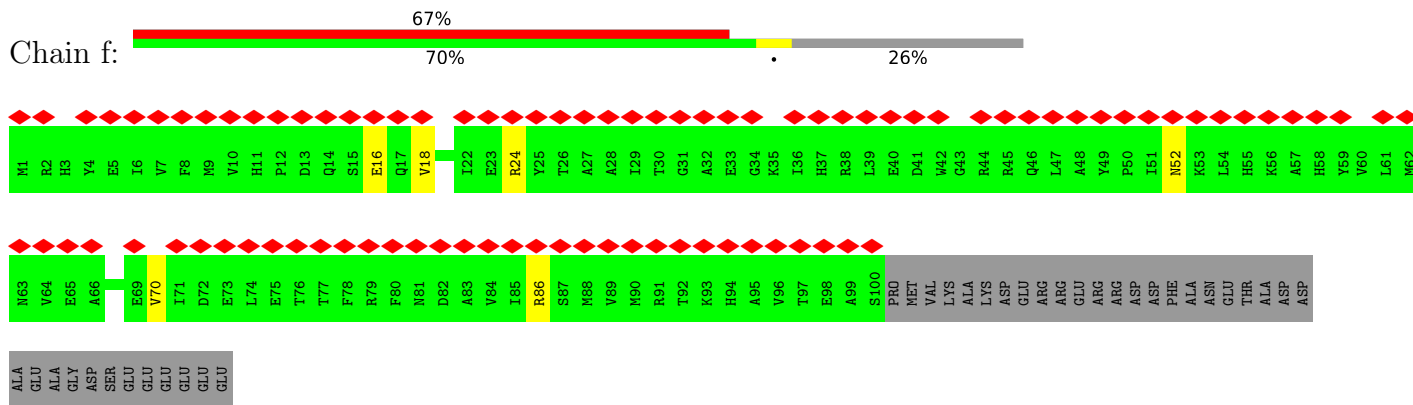
• Molecule 36: 30S ribosomal protein S5



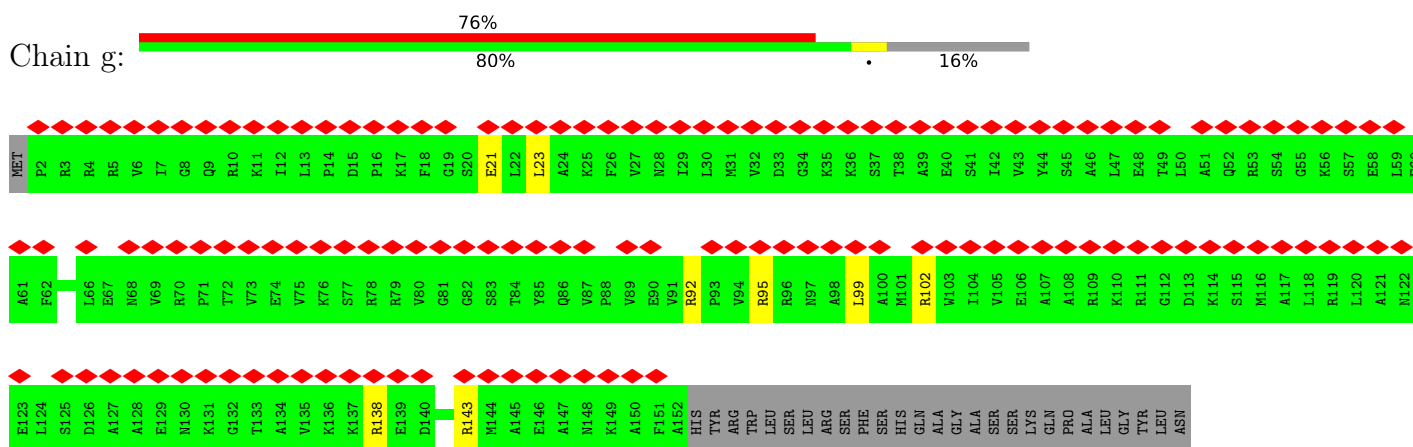
Chain e:



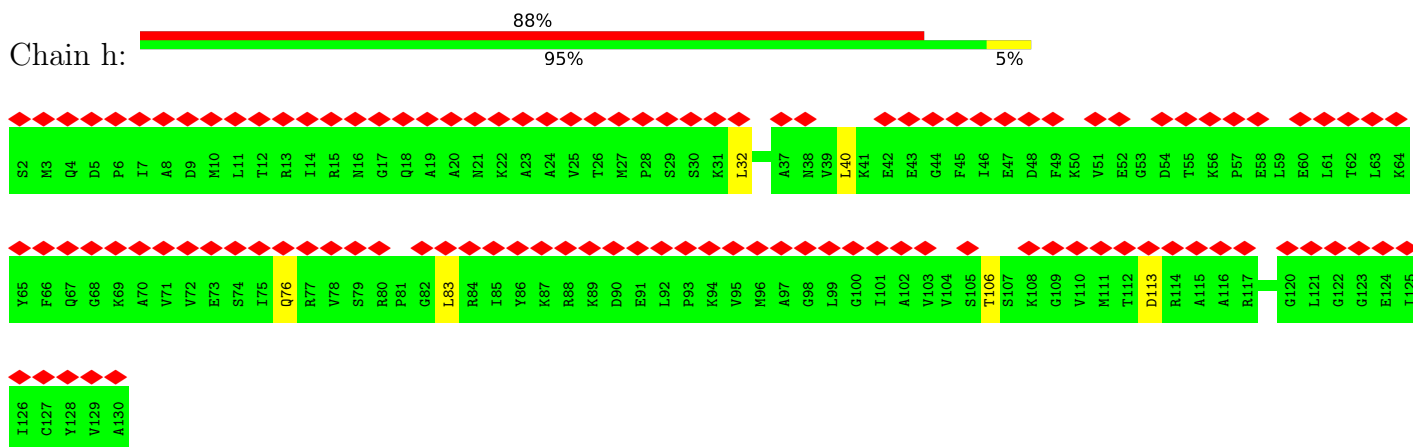
• Molecule 37: 30S ribosomal protein S6



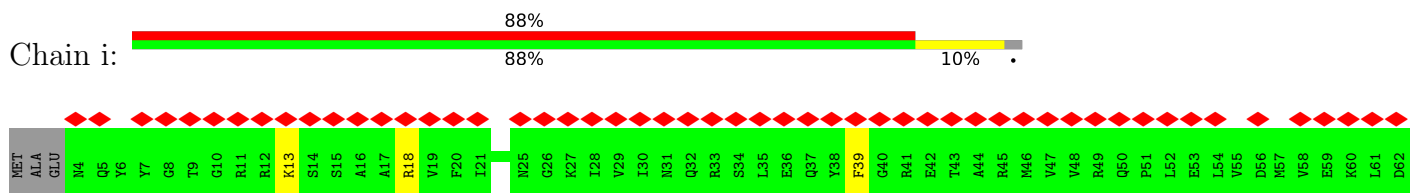
• Molecule 38: 30S ribosomal protein S7

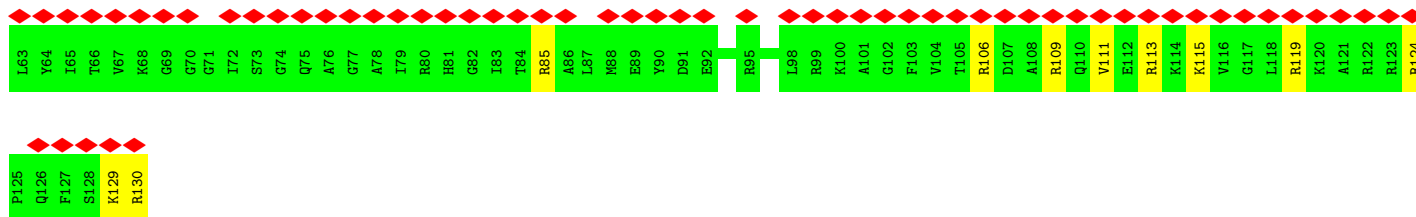


• Molecule 39: 30S ribosomal protein S8

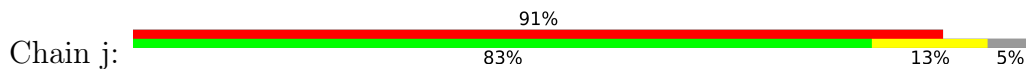


• Molecule 40: 30S ribosomal protein S9





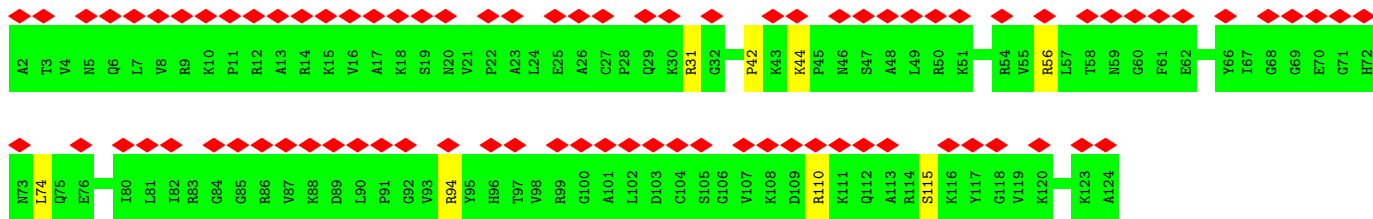
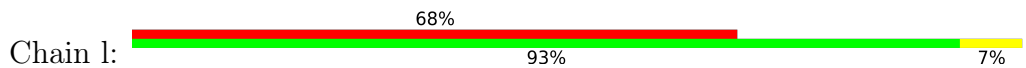
- Molecule 41: 30S ribosomal protein S10



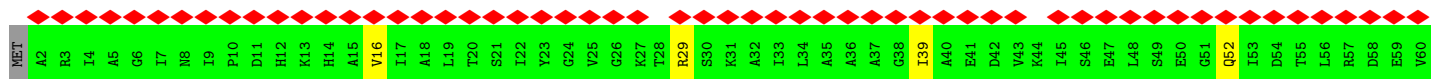
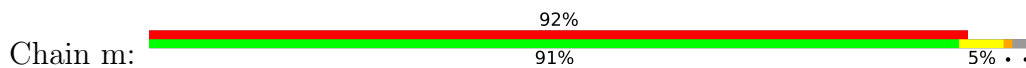
- Molecule 42: 30S ribosomal protein S11

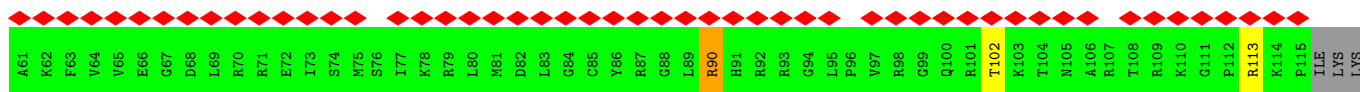


- Molecule 43: 30S ribosomal protein S12

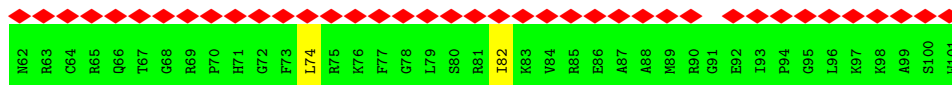
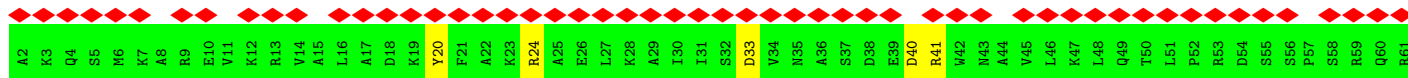
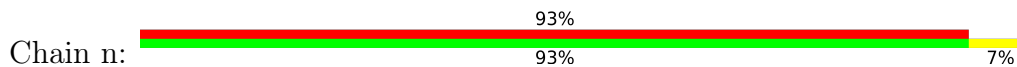


- Molecule 44: 30S ribosomal protein S13

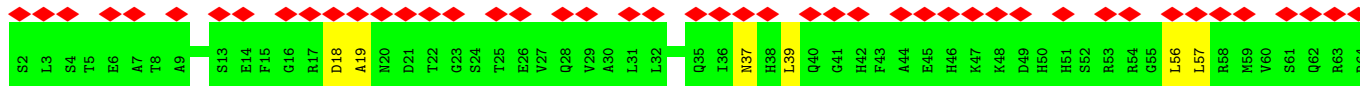
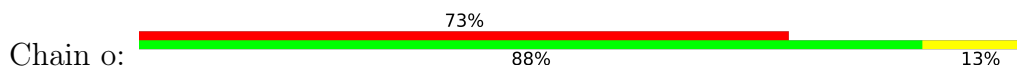




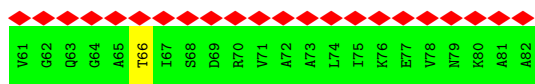
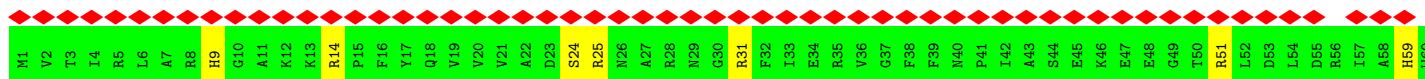
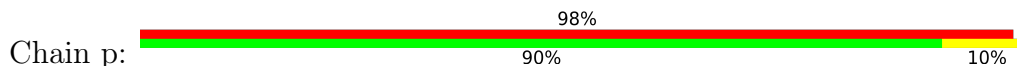
• Molecule 45: 30S ribosomal protein S14



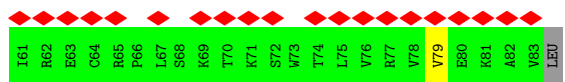
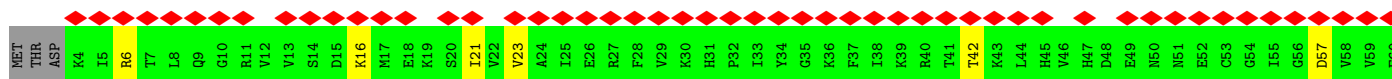
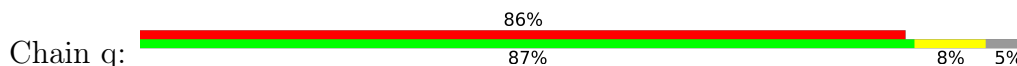
• Molecule 46: 30S ribosomal protein S15



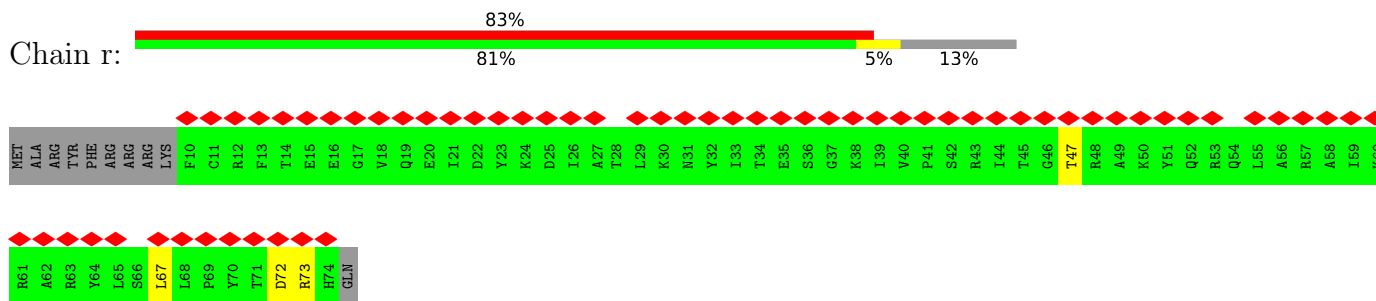
• Molecule 47: 30S ribosomal protein S16



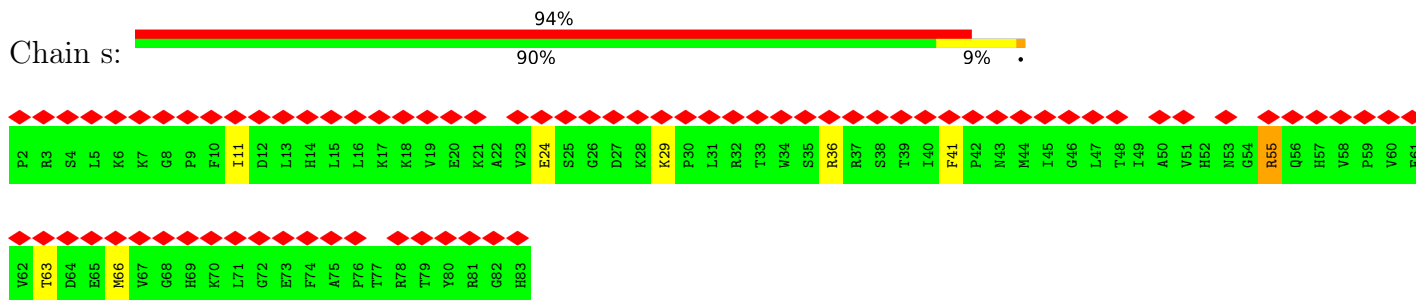
• Molecule 48: 30S ribosomal protein S17



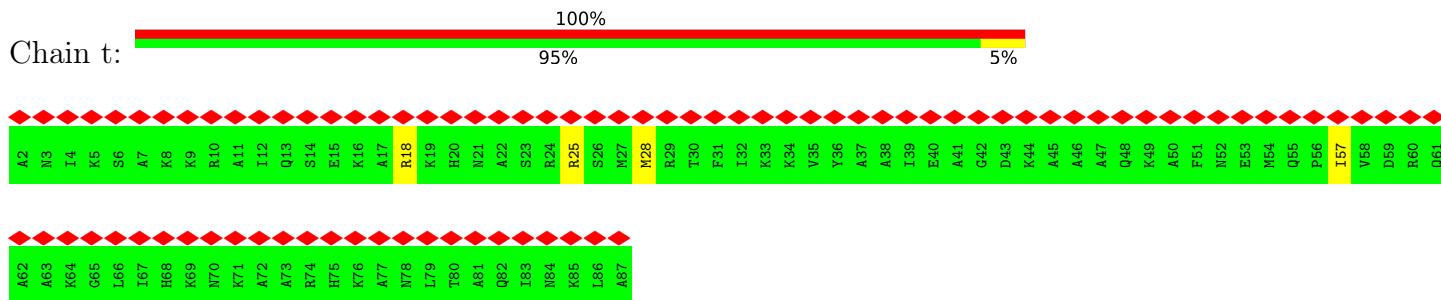
• Molecule 49: 30S ribosomal protein S18



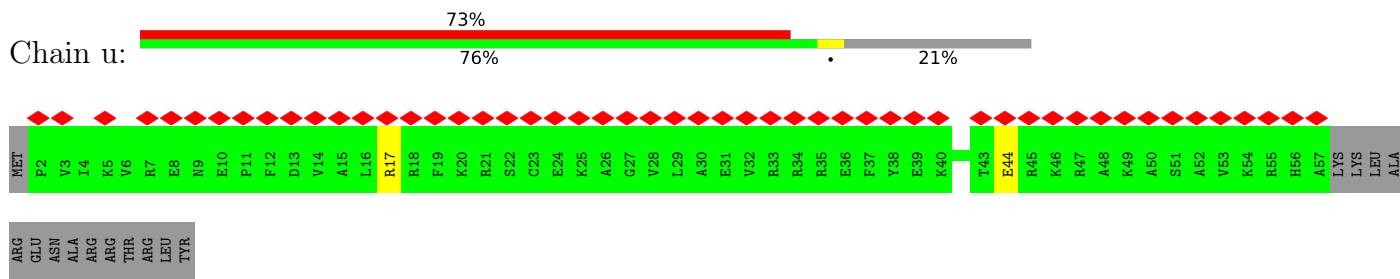
• Molecule 50: 30S ribosomal protein S19



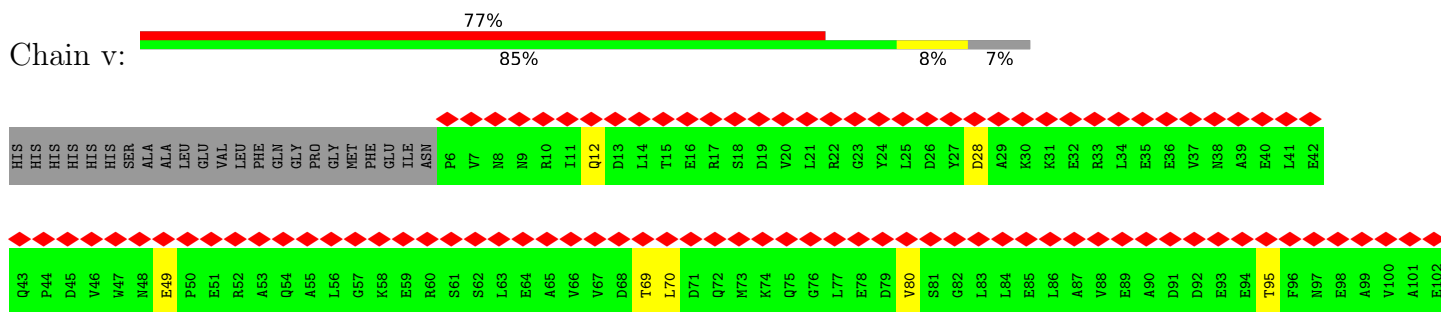
• Molecule 51: 30S ribosomal protein S20

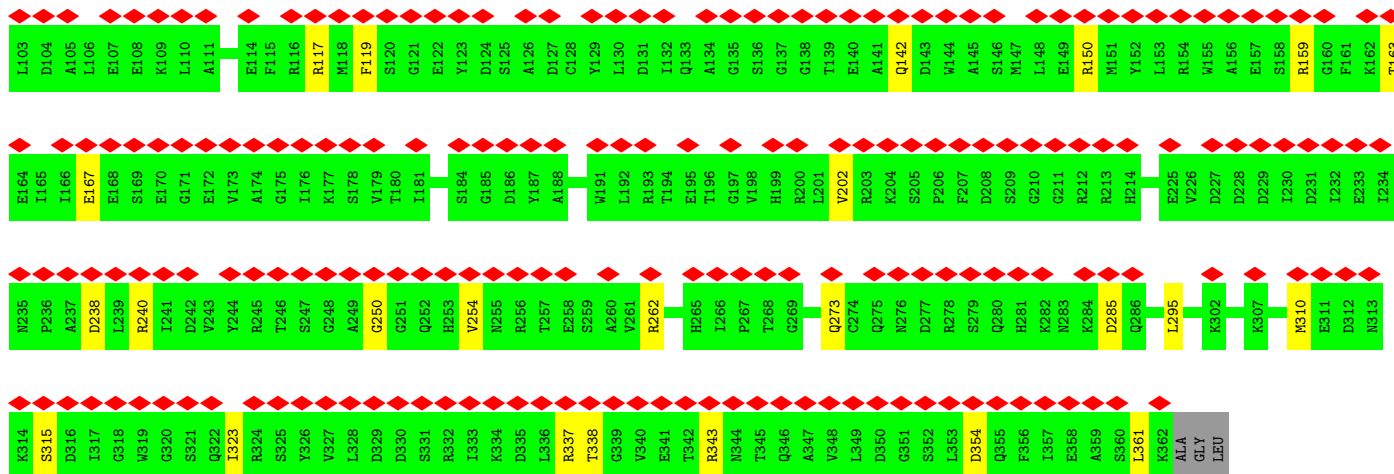


• Molecule 52: 30S ribosomal protein S21

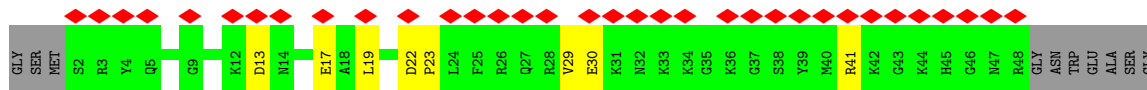


• Molecule 53: Peptide chain release factor 2

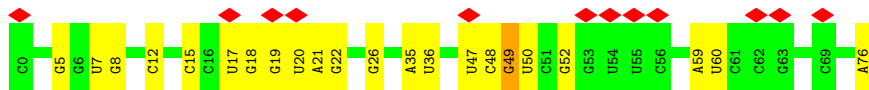




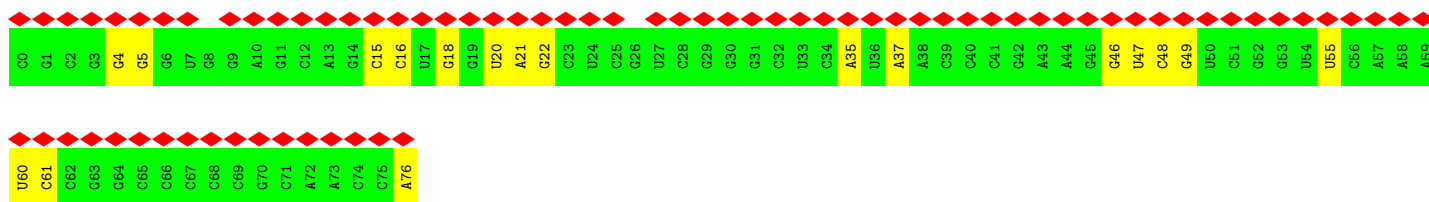
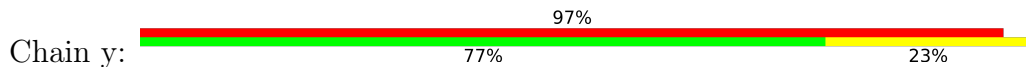
• Molecule 54: Alternative ribosome-rescue factor A



• 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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1730	C	C2'-C3'-O3'	5.50	122.49	113.70
26	0	25	LEU	CA-CB-CG	5.35	127.61	115.30
25	Z	18	LEU	CA-CB-CG	5.15	127.15	115.30

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
10	K	81	ILE
14	O	67	PHE
18	S	51	VAL
34	c	4	LYS
37	f	52	ASN
41	j	36	VAL
41	j	57	VAL
3	C	255	LYS
9	J	92	PRO
19	T	72	THR
21	V	90	GLY
26	0	4	THR
33	b	126	PHE
36	e	78	ASN
40	i	13	LYS
40	i	111	VAL
41	j	94	ALA
4	D	206	ALA
6	F	21	ASN
8	H	15	LEU
8	H	72	ILE
12	M	86	GLU
40	i	109	ARG

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Mol	Chain	Res	Type
53	v	250	GLY
3	C	69	ARG
6	F	176	PRO
6	F	177	PHE
18	S	80	ARG
23	X	76	ASN
25	Z	37	LEU
42	k	39	GLY
46	o	19	ALA
9	J	18	ASN
15	P	34	HIS
20	U	10	VAL
28	2	5	ILE
43	l	42	PRO
36	e	44	GLY
54	w	23	PRO
9	J	22	PRO
9	J	31	GLY
34	c	108	LYS
5	E	77	ILE
9	J	12	VAL
50	s	29	LYS
20	U	14	PRO

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (346) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	13	ARG
3	C	33	LEU
3	C	51	THR
3	C	52	ARG
3	C	63	ARG
3	C	72	ASP
3	C	80	ARG
3	C	133	ARG
3	C	135	ILE
3	C	142	HIS
3	C	156	ARG
3	C	164	ILE
3	C	175	ARG
3	C	176	LEU
3	C	182	ARG
3	C	221	ARG
3	C	264	ASP
3	C	269	ARG

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Mol	Chain	Res	Type
4	D	5	VAL
4	D	12	THR
4	D	45	TYR
4	D	50	VAL
4	D	77	ARG
4	D	121	THR
4	D	141	ARG
4	D	142	VAL
4	D	159	LYS
4	D	179	ARG
4	D	200	ASP
5	E	21	ARG
5	E	100	MET
5	E	107	SER
5	E	138	LEU
5	E	189	THR
5	E	193	VAL
6	F	6	ASP
6	F	16	LEU
6	F	22	TYR
6	F	52	ASN
6	F	71	ARG
6	F	74	VAL
6	F	95	ARG
6	F	108	VAL
6	F	135	GLN
6	F	152	LEU
6	F	155	THR
6	F	170	LEU
7	G	45	HIS
7	G	50	LEU
7	G	89	LEU
7	G	98	VAL
7	G	148	LEU
8	H	1	MET
8	H	9	VAL
8	H	27	ARG
8	H	96	THR
8	H	124	THR
9	J	8	VAL
9	J	37	PHE
9	J	60	VAL

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Mol	Chain	Res	Type
9	J	79	LEU
9	J	133	ARG
9	J	137	LEU
10	K	28	LEU
10	K	81	ILE
11	L	25	LEU
11	L	29	HIS
11	L	31	ARG
11	L	57	VAL
11	L	71	ARG
11	L	84	CYS
11	L	85	VAL
11	L	116	ILE
12	M	23	ILE
12	M	27	LEU
12	M	46	VAL
12	M	48	ARG
12	M	110	VAL
12	M	126	ARG
12	M	132	ARG
13	N	44	ARG
13	N	60	GLN
13	N	66	ARG
13	N	74	THR
13	N	86	LYS
13	N	119	LEU
14	O	15	SER
14	O	37	THR
14	O	70	THR
14	O	79	LEU
14	O	90	ARG
15	P	7	ARG
15	P	21	LEU
15	P	30	ARG
15	P	36	TYR
15	P	53	THR
15	P	83	LEU
15	P	84	GLU
15	P	106	LEU
16	Q	21	ARG
16	Q	33	VAL
16	Q	88	ARG

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Mol	Chain	Res	Type
16	Q	93	ARG
16	Q	97	LEU
16	Q	109	ARG
17	R	11	ARG
17	R	28	ARG
17	R	30	ARG
17	R	40	ILE
17	R	51	ARG
17	R	53	ARG
17	R	74	ILE
17	R	83	LEU
18	S	40	MET
18	S	54	VAL
18	S	80	ARG
19	T	46	LEU
20	U	60	THR
20	U	77	ARG
21	V	6	ARG
21	V	9	ASP
21	V	72	ILE
21	V	81	ASP
21	V	82	ARG
22	W	9	ARG
22	W	12	GLN
22	W	18	ARG
22	W	29	ILE
22	W	43	ASP
22	W	51	GLN
22	W	61	LEU
22	W	64	VAL
22	W	82	TYR
23	X	25	ARG
23	X	51	VAL
23	X	56	ASP
23	X	69	PHE
24	Y	18	ARG
24	Y	23	ASN
24	Y	33	LEU
24	Y	37	ARG
24	Y	46	PHE
24	Y	60	ASP
24	Y	78	TYR

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Mol	Chain	Res	Type
25	Z	56	LEU
27	1	9	THR
27	1	39	LEU
28	2	32	GLU
33	b	19	GLN
33	b	35	ARG
33	b	39	HIS
33	b	51	ASN
33	b	87	CYS
33	b	97	LEU
33	b	102	THR
33	b	106	THR
33	b	114	LEU
33	b	125	THR
33	b	137	ARG
33	b	139	ARG
33	b	179	LEU
33	b	204	ASP
34	c	25	ASN
34	c	43	LEU
34	c	59	ARG
34	c	65	ARG
34	c	72	ARG
34	c	75	ILE
34	c	87	LEU
34	c	90	VAL
34	c	93	ASP
34	c	106	VAL
34	c	110	GLU
34	c	140	ASN
34	c	169	ARG
34	c	176	HIS
34	c	178	LEU
34	c	179	ARG
34	c	206	GLU
35	d	3	ARG
35	d	28	ILE
35	d	35	GLU
35	d	44	ARG
35	d	55	LEU
35	d	58	LYS
35	d	73	ARG

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Mol	Chain	Res	Type
35	d	91	LEU
35	d	93	LEU
35	d	97	ARG
35	d	116	GLN
35	d	141	ASP
35	d	159	LEU
35	d	191	LEU
36	e	31	PHE
36	e	34	THR
36	e	45	ARG
36	e	69	ARG
36	e	76	LEU
36	e	90	THR
36	e	93	ARG
36	e	120	VAL
36	e	123	VAL
36	e	131	THR
36	e	136	VAL
36	e	165	LEU
37	f	16	GLU
37	f	18	VAL
37	f	24	ARG
37	f	70	VAL
37	f	86	ARG
38	g	21	GLU
38	g	23	LEU
38	g	92	ARG
38	g	95	ARG
38	g	99	LEU
38	g	102	ARG
38	g	138	ARG
38	g	143	ARG
39	h	32	LEU
39	h	40	LEU
39	h	76	GLN
39	h	83	LEU
39	h	106	THR
39	h	113	ASP
40	i	18	ARG
40	i	39	PHE
40	i	85	ARG
40	i	106	ARG

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Mol	Chain	Res	Type
40	i	113	ARG
40	i	115	LYS
40	i	119	ARG
40	i	124	ARG
40	i	129	LYS
40	i	130	ARG
41	j	7	ARG
41	j	9	ARG
41	j	10	LEU
41	j	16	ARG
41	j	31	ARG
41	j	37	ARG
41	j	53	ILE
41	j	68	ARG
41	j	73	LEU
41	j	102	LEU
42	k	53	ARG
42	k	96	THR
43	l	31	ARG
43	l	44	LYS
43	l	56	ARG
43	l	74	LEU
43	l	94	ARG
43	l	110	ARG
43	l	115	SER
44	m	16	VAL
44	m	29	ARG
44	m	39	ILE
44	m	52	GLN
44	m	90	ARG
44	m	102	THR
44	m	113	ARG
45	n	20	TYR
45	n	24	ARG
45	n	33	ASP
45	n	40	ASP
45	n	41	ARG
45	n	74	LEU
45	n	82	ILE
46	o	18	ASP
46	o	37	ASN
46	o	39	LEU

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Mol	Chain	Res	Type
46	o	56	LEU
46	o	57	LEU
46	o	73	LYS
46	o	75	VAL
46	o	84	ARG
46	o	88	ARG
46	o	89	ARG
47	p	9	HIS
47	p	14	ARG
47	p	24	SER
47	p	25	ARG
47	p	31	ARG
47	p	51	ARG
47	p	59	HIS
47	p	66	THR
48	q	6	ARG
48	q	16	LYS
48	q	21	ILE
48	q	23	VAL
48	q	42	THR
48	q	57	ASP
48	q	79	VAL
49	r	47	THR
49	r	67	LEU
49	r	72	ASP
49	r	73	ARG
50	s	11	ILE
50	s	24	GLU
50	s	36	ARG
50	s	41	PHE
50	s	55	ARG
50	s	63	THR
50	s	66	MET
51	t	18	ARG
51	t	25	ARG
51	t	28	MET
51	t	57	ILE
52	u	17	ARG
52	u	44	GLU
53	v	12	GLN
53	v	28	ASP
53	v	49	GLU

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Mol	Chain	Res	Type
53	v	69	THR
53	v	70	LEU
53	v	80	VAL
53	v	95	THR
53	v	117	ARG
53	v	119	PHE
53	v	142	GLN
53	v	150	ARG
53	v	159	ARG
53	v	163	THR
53	v	167	GLU
53	v	202	VAL
53	v	238	ASP
53	v	240	ARG
53	v	254	VAL
53	v	262	ARG
53	v	273	GLN
53	v	285	ASP
53	v	295	LEU
53	v	310	MET
53	v	315	SER
53	v	323	ILE
53	v	337	ARG
53	v	338	THR
53	v	343	ARG
53	v	354	ASP
53	v	361	LEU
54	w	13	ASP
54	w	17	GLU
54	w	19	LEU
54	w	22	ASP
54	w	29	VAL
54	w	30	GLU
54	w	41	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	44	ASN
3	C	60	GLN
4	D	173	GLN
5	E	62	GLN

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Mol	Chain	Res	Type
5	E	90	GLN
7	G	22	GLN
7	G	111	HIS
7	G	116	GLN
8	H	135	HIS
12	M	38	GLN
14	O	16	HIS
14	O	62	ASN
16	Q	3	ASN
17	R	20	GLN
17	R	72	ASN
18	S	12	HIS
18	S	18	GLN
19	T	15	GLN
19	T	61	ASN
21	V	40	ASN
21	V	46	GLN
22	W	44	HIS
22	W	49	ASN
25	Z	39	GLN
34	c	123	GLN
35	d	36	GLN
36	e	73	ASN
36	e	89	HIS
36	e	135	ASN
36	e	146	ASN
37	f	52	ASN
37	f	81	ASN
38	g	86	GLN
38	g	148	ASN
42	k	119	ASN
43	l	6	GLN
43	l	29	GLN
47	p	63	GLN
48	q	51	ASN
49	r	54	GLN
53	v	43	GLN
53	v	214	HIS
53	v	253	HIS
53	v	283	ASN
53	v	286	GLN

5.3.3 RNA 

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%)

All (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
1	A	34	U
1	A	35	G
1	A	39	G
1	A	43	G
1	A	45	G
1	A	46	G
1	A	49	A
1	A	51	G
1	A	55	G
1	A	60	G
1	A	61	C
1	A	63	A
1	A	69	C
1	A	71	A
1	A	73	A
1	A	74	A
1	A	75	G
1	A	83	A
1	A	84	A
1	A	86	G
1	A	88	G
1	A	92	U
1	A	93	G
1	A	96	C
1	A	101	A

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Mol	Chain	Res	Type
1	A	102	U
1	A	103	A
1	A	110	G
1	A	114	U
1	A	118	A
1	A	119	A
1	A	120	U
1	A	122	G
1	A	125	A
1	A	127	A
1	A	131	A
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	142	A
1	A	150	U
1	A	157	C
1	A	163	C
1	A	179	C
1	A	181	A
1	A	184	C
1	A	196	A
1	A	199	A
1	A	204	A
1	A	205	G
1	A	215	G
1	A	216	A
1	A	222	A
1	A	224	U
1	A	228	C
1	A	230	G
1	A	233	A
1	A	239	C
1	A	241	A
1	A	248	G
1	A	249	C
1	A	252	G
1	A	261	G
1	A	264	C
1	A	265	A
1	A	266	G

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Mol	Chain	Res	Type
1	A	271	G
1	A	272	A
1	A	276	U
1	A	278	A
1	A	279	A
1	A	285	G
1	A	291	G
1	A	295	G
1	A	302	C
1	A	311	A
1	A	312	G
1	A	313	G
1	A	318	C
1	A	322	A
1	A	323	C
1	A	329	G
1	A	330	A
1	A	331	C
1	A	346	A
1	A	352	A
1	A	353	C
1	A	356	G
1	A	361	G
1	A	362	A
1	A	367	G
1	A	370	G
1	A	371	A
1	A	372	G
1	A	373	U
1	A	386	G
1	A	387	U
1	A	399	U
1	A	402	A
1	A	403	U
1	A	404	A
1	A	405	U
1	A	408	G
1	A	411	G
1	A	421	C
1	A	424	G
1	A	425	G
1	A	427	U

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Mol	Chain	Res	Type
1	A	431	U
1	A	435	C
1	A	442	G
1	A	443	A
1	A	444	C
1	A	451	U
1	A	454	A
1	A	455	C
1	A	457	A
1	A	467	G
1	A	474	G
1	A	475	C
1	A	476	G
1	A	479	A
1	A	481	G
1	A	490	C
1	A	491	G
1	A	501	A
1	A	504	A
1	A	505	A
1	A	506	G
1	A	512	G
1	A	513	A
1	A	516	C
1	A	518	G
1	A	519	U
1	A	527	C
1	A	528	A
1	A	529	A
1	A	531	C
1	A	532	A
1	A	544	C
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	551	G
1	A	555	G
1	A	562	U
1	A	563	A
1	A	565	C
1	A	566	U

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Mol	Chain	Res	Type
1	A	568	U
1	A	573	U
1	A	575	A
1	A	577	G
1	A	580	U
1	A	588	U
1	A	592	A
1	A	593	U
1	A	601	C
1	A	603	A
1	A	610	C
1	A	613	A
1	A	614	A
1	A	615	U
1	A	621	A
1	A	627	A
1	A	637	A
1	A	638	G
1	A	645	C
1	A	647	G
1	A	651	G
1	A	653	U
1	A	654	A
1	A	655	A
1	A	659	G
1	A	664	G
1	A	668	A
1	A	670	A
1	A	675	A
1	A	677	A
1	A	684	G
1	A	686	U
1	A	691	C
1	A	694	U
1	A	702	U
1	A	710	U
1	A	717	C
1	A	726	G
1	A	728	G
1	A	729	G
1	A	730	A
1	A	731	C

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Mol	Chain	Res	Type
1	A	734	A
1	A	738	G
1	A	742	A
1	A	743	A
1	A	746	PSU
1	A	747	5MU
1	A	757	G
1	A	763	G
1	A	764	A
1	A	765	C
1	A	775	G
1	A	776	G
1	A	777	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	788	A
1	A	792	A
1	A	799	G
1	A	800	A
1	A	805	G
1	A	811	U
1	A	812	C
1	A	819	A
1	A	821	A
1	A	827	U
1	A	828	U
1	A	831	G
1	A	845	A
1	A	846	U
1	A	847	U
1	A	850	U
1	A	856	G
1	A	858	G
1	A	859	G
1	A	869	G
1	A	877	A
1	A	878	A
1	A	881	G
1	A	882	G
1	A	883	G
1	A	886	A

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Mol	Chain	Res	Type
1	A	887	A
1	A	888	C
1	A	889	C
1	A	890	C
1	A	894	U
1	A	895	U
1	A	896	A
1	A	897	C
1	A	907	G
1	A	910	A
1	A	914	G
1	A	915	C
1	A	918	A
1	A	926	G
1	A	931	U
1	A	932	U
1	A	941	A
1	A	946	C
1	A	953	G
1	A	957	C
1	A	958	U
1	A	961	C
1	A	964	C
1	A	965	C
1	A	968	C
1	A	973	A
1	A	974	G
1	A	983	A
1	A	984	A
1	A	988	A
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	997	G
1	A	1007	C
1	A	1008	A
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1017	G
1	A	1021	A

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Mol	Chain	Res	Type
1	A	1022	G
1	A	1023	U
1	A	1024	G
1	A	1025	G
1	A	1026	G
1	A	1033	U
1	A	1034	G
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1051	G
1	A	1052	C
1	A	1054	A
1	A	1059	G
1	A	1065	U
1	A	1066	U
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1073	A
1	A	1074	G
1	A	1075	C
1	A	1076	C
1	A	1077	A
1	A	1078	U
1	A	1080	A
1	A	1083	U
1	A	1085	A
1	A	1087	G
1	A	1088	A
1	A	1089	A
1	A	1096	A
1	A	1097	U
1	A	1098	A
1	A	1101	U
1	A	1102	C
1	A	1106	G
1	A	1111	A
1	A	1112	G
1	A	1118	C
1	A	1119	U

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Mol	Chain	Res	Type
1	A	1121	C
1	A	1126	A
1	A	1127	A
1	A	1131	G
1	A	1132	U
1	A	1133	A
1	A	1134	A
1	A	1135	C
1	A	1136	G
1	A	1142	A
1	A	1143	A
1	A	1144	A
1	A	1151	A
1	A	1155	A
1	A	1156	A
1	A	1165	A
1	A	1170	C
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1179	G
1	A	1180	U
1	A	1182	G
1	A	1186	G
1	A	1187	G
1	A	1188	U
1	A	1195	G
1	A	1205	A
1	A	1206	G
1	A	1210	G
1	A	1212	G
1	A	1218	G
1	A	1223	G
1	A	1227	G
1	A	1236	G
1	A	1238	G
1	A	1240	U
1	A	1244	A
1	A	1247	A
1	A	1248	G
1	A	1249	U

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Mol	Chain	Res	Type
1	A	1252	G
1	A	1253	A
1	A	1256	G
1	A	1263	U
1	A	1265	A
1	A	1266	G
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1277	G
1	A	1278	C
1	A	1288	G
1	A	1289	C
1	A	1294	U
1	A	1300	G
1	A	1301	A
1	A	1302	A
1	A	1306	C
1	A	1312	U
1	A	1313	U
1	A	1314	C
1	A	1315	C
1	A	1320	C
1	A	1321	A
1	A	1326	U
1	A	1329	U
1	A	1341	G
1	A	1344	U
1	A	1345	C
1	A	1352	U
1	A	1360	G
1	A	1365	A
1	A	1368	G
1	A	1371	G
1	A	1379	U
1	A	1380	G
1	A	1383	A
1	A	1395	A
1	A	1398	C
1	A	1403	A
1	A	1404	C
1	A	1407	G

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Mol	Chain	Res	Type
1	A	1408	G
1	A	1409	U
1	A	1416	G
1	A	1417	C
1	A	1419	A
1	A	1420	A
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1429	G
1	A	1433	A
1	A	1434	A
1	A	1437	C
1	A	1438	U
1	A	1444	G
1	A	1449	G
1	A	1451	C
1	A	1453	A
1	A	1455	G
1	A	1456	G
1	A	1458	U
1	A	1460	U
1	A	1461	C
1	A	1466	U
1	A	1468	U
1	A	1471	G
1	A	1478	G
1	A	1482	G
1	A	1486	U
1	A	1488	C
1	A	1490	A
1	A	1492	G
1	A	1493	C
1	A	1494	A
1	A	1497	U
1	A	1502	A
1	A	1503	A
1	A	1508	A
1	A	1515	A
1	A	1522	A
1	A	1523	U
1	A	1531	C

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Mol	Chain	Res	Type
1	A	1532	A
1	A	1533	C
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1550	C
1	A	1555	G
1	A	1558	C
1	A	1566	A
1	A	1567	G
1	A	1569	A
1	A	1578	U
1	A	1580	A
1	A	1581	G
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1586	A
1	A	1592	C
1	A	1597	A
1	A	1599	U
1	A	1607	C
1	A	1608	A
1	A	1610	A
1	A	1613	G
1	A	1619	G
1	A	1627	G
1	A	1634	A
1	A	1638	C
1	A	1639	C
1	A	1643	G
1	A	1644	C
1	A	1646	C
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1652	A
1	A	1654	A
1	A	1660	G
1	A	1664	A
1	A	1666	G

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Mol	Chain	Res	Type
1	A	1667	G
1	A	1669	A
1	A	1674	G
1	A	1675	C
1	A	1695	G
1	A	1713	A
1	A	1715	G
1	A	1721	G
1	A	1724	G
1	A	1729	U
1	A	1730	C
1	A	1731	G
1	A	1732	C
1	A	1733	G
1	A	1742	U
1	A	1758	U
1	A	1759	A
1	A	1764	C
1	A	1773	A
1	A	1782	U
1	A	1786	A
1	A	1791	A
1	A	1794	A
1	A	1800	C
1	A	1801	A
1	A	1808	A
1	A	1816	C
1	A	1821	A
1	A	1829	A
1	A	1835	2MG
1	A	1848	A
1	A	1864	U
1	A	1865	U
1	A	1866	A
1	A	1869	G
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1875	G
1	A	1876	A
1	A	1882	U

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Mol	Chain	Res	Type
1	A	1884	G
1	A	1885	A
1	A	1900	A
1	A	1901	A
1	A	1906	G
1	A	1907	G
1	A	1913	A
1	A	1914	C
1	A	1929	G
1	A	1930	G
1	A	1931	U
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1939	5MU
1	A	1940	U
1	A	1944	U
1	A	1955	U
1	A	1964	G
1	A	1965	C
1	A	1966	A
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1981	A
1	A	1982	U
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	1997	C
1	A	2000	C
1	A	2002	G
1	A	2004	G
1	A	2006	C
1	A	2016	U
1	A	2018	G
1	A	2020	A
1	A	2022	U
1	A	2023	C
1	A	2027	G
1	A	2030	A

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Mol	Chain	Res	Type
1	A	2031	A
1	A	2034	U
1	A	2036	C
1	A	2043	C
1	A	2046	G
1	A	2049	G
1	A	2050	C
1	A	2052	A
1	A	2055	C
1	A	2056	G
1	A	2057	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2068	U
1	A	2069	G
1	A	2070	A
1	A	2072	C
1	A	2074	U
1	A	2075	U
1	A	2077	A
1	A	2080	A
1	A	2087	G
1	A	2093	G
1	A	2095	A
1	A	2101	A
1	A	2102	G
1	A	2107	G
1	A	2110	G
1	A	2111	U
1	A	2113	U
1	A	2115	G
1	A	2116	G
1	A	2117	A
1	A	2118	U
1	A	2121	G
1	A	2122	U
1	A	2125	G
1	A	2130	U
1	A	2131	U
1	A	2132	U

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Mol	Chain	Res	Type
1	A	2134	A
1	A	2139	U
1	A	2142	A
1	A	2146	C
1	A	2147	A
1	A	2148	G
1	A	2150	C
1	A	2154	A
1	A	2157	G
1	A	2158	A
1	A	2159	G
1	A	2160	C
1	A	2162	G
1	A	2164	C
1	A	2165	C
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2178	C
1	A	2182	U
1	A	2183	A
1	A	2189	U
1	A	2193	G
1	A	2194	U
1	A	2198	A
1	A	2203	U
1	A	2204	G
1	A	2211	A
1	A	2212	A
1	A	2213	U
1	A	2214	C
1	A	2216	G
1	A	2221	G
1	A	2223	G
1	A	2225	A
1	A	2226	C
1	A	2234	G
1	A	2238	G
1	A	2243	U
1	A	2249	U
1	A	2250	G
1	A	2266	A

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Mol	Chain	Res	Type
1	A	2278	A
1	A	2279	G
1	A	2280	G
1	A	2282	G
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2288	A
1	A	2292	U
1	A	2297	A
1	A	2301	C
1	A	2305	U
1	A	2307	G
1	A	2309	A
1	A	2311	A
1	A	2319	G
1	A	2322	A
1	A	2325	G
1	A	2327	A
1	A	2331	G
1	A	2333	A
1	A	2335	A
1	A	2336	A
1	A	2339	C
1	A	2345	G
1	A	2347	C
1	A	2350	C
1	A	2353	G
1	A	2354	C
1	A	2355	G
1	A	2357	G
1	A	2361	G
1	A	2376	A
1	A	2383	G
1	A	2384	U
1	A	2385	C
1	A	2388	A
1	A	2391	G
1	A	2400	G
1	A	2402	U
1	A	2403	C
1	A	2406	A

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Mol	Chain	Res	Type
1	A	2408	U
1	A	2409	G
1	A	2410	G
1	A	2419	U
1	A	2423	U
1	A	2424	C
1	A	2425	A
1	A	2427	C
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2432	A
1	A	2434	A
1	A	2435	A
1	A	2436	G
1	A	2441	U
1	A	2445	2MG
1	A	2447	G
1	A	2448	A
1	A	2457	PSU
1	A	2464	G
1	A	2468	A
1	A	2469	A
1	A	2470	G
1	A	2476	A
1	A	2480	C
1	A	2484	G
1	A	2487	G
1	A	2490	G
1	A	2491	U
1	A	2492	U
1	A	2494	G
1	A	2498	OMC
1	A	2500	U
1	A	2502	G
1	A	2503	A
1	A	2504	PSU
1	A	2505	G
1	A	2506	U
1	A	2511	U
1	A	2513	A

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Mol	Chain	Res	Type
1	A	2517	C
1	A	2518	A
1	A	2519	U
1	A	2520	C
1	A	2528	U
1	A	2531	A
1	A	2535	G
1	A	2549	G
1	A	2554	U
1	A	2561	U
1	A	2562	U
1	A	2566	A
1	A	2567	G
1	A	2569	G
1	A	2573	C
1	A	2574	G
1	A	2578	G
1	A	2582	G
1	A	2585	U
1	A	2602	A
1	A	2603	G
1	A	2608	G
1	A	2609	U
1	A	2613	U
1	A	2614	A
1	A	2615	U
1	A	2621	G
1	A	2623	G
1	A	2629	U
1	A	2632	A
1	A	2634	A
1	A	2636	C
1	A	2639	A
1	A	2645	G
1	A	2646	C
1	A	2647	U
1	A	2656	U
1	A	2658	C
1	A	2663	G
1	A	2665	A
1	A	2673	G
1	A	2682	A

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Mol	Chain	Res	Type
1	A	2685	G
1	A	2689	U
1	A	2690	U
1	A	2713	U
1	A	2714	G
1	A	2716	C
1	A	2718	G
1	A	2723	C
1	A	2725	A
1	A	2726	A
1	A	2728	U
1	A	2731	G
1	A	2732	G
1	A	2733	A
1	A	2735	G
1	A	2739	U
1	A	2744	G
1	A	2748	A
1	A	2750	A
1	A	2751	G
1	A	2752	C
1	A	2754	U
1	A	2756	U
1	A	2761	A
1	A	2762	C
1	A	2763	G
1	A	2765	A
1	A	2776	A
1	A	2777	G
1	A	2778	A
1	A	2780	G
1	A	2784	U
1	A	2791	G
1	A	2792	A
1	A	2793	C
1	A	2794	C
1	A	2797	U
1	A	2800	A
1	A	2803	G
1	A	2805	C
1	A	2809	A
1	A	2813	A

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Mol	Chain	Res	Type
1	A	2816	G
1	A	2818	U
1	A	2820	A
1	A	2821	A
1	A	2823	A
1	A	2824	C
1	A	2830	C
1	A	2833	U
1	A	2835	A
1	A	2836	U
1	A	2848	G
1	A	2849	U
1	A	2854	G
1	A	2867	G
1	A	2873	A
1	A	2880	C
1	A	2883	A
1	A	2884	U
1	A	2885	G
1	A	2886	A
1	A	2891	U
1	A	2892	G
1	A	2898	U
1	A	2899	A
1	A	2902	C
1	A	2903	U
1	A	2904	U
2	B	7	G
2	B	9	G
2	B	12	C
2	B	14	U
2	B	15	A
2	B	17	C
2	B	22	U
2	B	24	G
2	B	29	A
2	B	30	C
2	B	34	A
2	B	35	C
2	B	40	U
2	B	41	G
2	B	42	C

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Mol	Chain	Res	Type
2	B	44	G
2	B	47	C
2	B	56	G
2	B	58	A
2	B	64	G
2	B	66	A
2	B	68	C
2	B	83	G
2	B	86	G
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	99	A
2	B	105	G
2	B	108	A
2	B	109	A
2	B	117	G
2	B	118	C
2	B	119	A
32	a	3	A
32	a	4	U
32	a	6	G
32	a	9	G
32	a	11	G
32	a	13	U
32	a	18	C
32	a	22	G
32	a	25	C
32	a	32	A
32	a	33	A
32	a	43	C
32	a	47	C
32	a	48	C
32	a	50	A
32	a	51	A
32	a	54	C
32	a	58	C
32	a	60	A
32	a	65	A
32	a	66	A
32	a	70	U

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Mol	Chain	Res	Type
32	a	71	A
32	a	72	A
32	a	82	G
32	a	83	C
32	a	84	U
32	a	86	G
32	a	87	C
32	a	88	U
32	a	92	U
32	a	93	U
32	a	94	G
32	a	95	C
32	a	99	C
32	a	100	G
32	a	101	A
32	a	104	G
32	a	105	G
32	a	108	G
32	a	109	A
32	a	110	C
32	a	114	U
32	a	119	A
32	a	120	A
32	a	122	G
32	a	126	G
32	a	127	G
32	a	128	G
32	a	129	A
32	a	130	A
32	a	131	A
32	a	132	C
32	a	133	U
32	a	134	G
32	a	137	U
32	a	141	G
32	a	142	G
32	a	144	G
32	a	145	G
32	a	146	G
32	a	149	A
32	a	158	G
32	a	161	A

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Mol	Chain	Res	Type
32	a	163	C
32	a	164	G
32	a	165	G
32	a	168	G
32	a	169	C
32	a	171	A
32	a	173	U
32	a	182	A
32	a	184	G
32	a	187	G
32	a	191	G
32	a	195	A
32	a	197	A
32	a	202	G
32	a	203	G
32	a	204	G
32	a	205	A
32	a	207	C
32	a	209	U
32	a	210	C
32	a	211	G
32	a	212	G
32	a	213	G
32	a	214	C
32	a	217	C
32	a	219	U
32	a	226	G
32	a	231	U
32	a	232	G
32	a	235	C
32	a	240	G
32	a	245	U
32	a	247	G
32	a	251	G
32	a	253	A
32	a	256	U
32	a	260	G
32	a	261	U
32	a	264	C
32	a	266	G
32	a	267	C
32	a	279	A

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Mol	Chain	Res	Type
32	a	281	G
32	a	289	G
32	a	298	A
32	a	300	A
32	a	301	G
32	a	306	A
32	a	308	C
32	a	315	A
32	a	316	C
32	a	321	A
32	a	322	C
32	a	328	C
32	a	329	A
32	a	332	G
32	a	346	G
32	a	350	G
32	a	351	G
32	a	352	C
32	a	354	G
32	a	356	A
32	a	362	G
32	a	367	U
32	a	368	U
32	a	369	G
32	a	370	C
32	a	371	A
32	a	372	C
32	a	373	A
32	a	377	G
32	a	378	G
32	a	380	G
32	a	382	A
32	a	390	U
32	a	392	C
32	a	397	A
32	a	398	U
32	a	406	G
32	a	408	A
32	a	412	A
32	a	413	G
32	a	414	A
32	a	421	U

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Mol	Chain	Res	Type
32	a	422	C
32	a	423	G
32	a	424	G
32	a	425	G
32	a	426	U
32	a	429	U
32	a	434	U
32	a	436	C
32	a	437	U
32	a	439	U
32	a	449	G
32	a	451	A
32	a	454	G
32	a	456	A
32	a	458	U
32	a	463	U
32	a	464	U
32	a	465	A
32	a	467	U
32	a	469	C
32	a	474	G
32	a	476	U
32	a	478	A
32	a	481	G
32	a	482	A
32	a	484	G
32	a	485	U
32	a	488	C
32	a	495	A
32	a	497	G
32	a	499	A
32	a	503	C
32	a	507	C
32	a	508	U
32	a	509	A
32	a	511	C
32	a	514	C
32	a	517	G
32	a	518	C
32	a	521	G
32	a	527	A
32	a	529	G

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Mol	Chain	Res	Type
32	a	531	U
32	a	532	A
32	a	533	A
32	a	536	C
32	a	542	G
32	a	547	A
32	a	549	C
32	a	555	U
32	a	559	A
32	a	561	U
32	a	562	U
32	a	563	A
32	a	564	C
32	a	572	A
32	a	573	A
32	a	575	G
32	a	576	C
32	a	577	G
32	a	579	A
32	a	585	G
32	a	588	G
32	a	596	A
32	a	605	U
32	a	606	G
32	a	607	A
32	a	615	G
32	a	619	U
32	a	620	C
32	a	625	U
32	a	626	G
32	a	632	U
32	a	633	G
32	a	641	U
32	a	642	A
32	a	647	C
32	a	653	U
32	a	654	G
32	a	656	G
32	a	661	G
32	a	665	A
32	a	667	G
32	a	671	G

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Mol	Chain	Res	Type
32	a	672	U
32	a	687	A
32	a	688	G
32	a	701	U
32	a	702	A
32	a	703	G
32	a	707	U
32	a	712	A
32	a	713	G
32	a	720	C
32	a	721	G
32	a	723	U
32	a	724	G
32	a	729	A
32	a	731	G
32	a	733	G
32	a	734	G
32	a	744	C
32	a	747	A
32	a	748	G
32	a	752	G
32	a	753	A
32	a	755	G
32	a	760	G
32	a	772	U
32	a	774	G
32	a	787	A
32	a	790	A
32	a	793	U
32	a	794	A
32	a	799	G
32	a	809	G
32	a	812	G
32	a	813	U
32	a	814	A
32	a	815	A
32	a	817	C
32	a	818	G
32	a	820	U
32	a	821	G
32	a	827	U
32	a	828	U

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Mol	Chain	Res	Type
32	a	829	G
32	a	832	G
32	a	841	C
32	a	844	G
32	a	845	A
32	a	846	G
32	a	849	G
32	a	851	G
32	a	854	U
32	a	862	C
32	a	873	A
32	a	874	G
32	a	880	C
32	a	884	U
32	a	899	C
32	a	902	G
32	a	913	A
32	a	914	A
32	a	919	A
32	a	922	G
32	a	931	C
32	a	934	C
32	a	935	A
32	a	939	G
32	a	941	G
32	a	943	U
32	a	960	U
32	a	961	U
32	a	965	U
32	a	966	2MG
32	a	967	5MC
32	a	968	A
32	a	969	A
32	a	971	G
32	a	974	A
32	a	975	A
32	a	976	G
32	a	977	A
32	a	983	A
32	a	986	U
32	a	990	C
32	a	992	U

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Mol	Chain	Res	Type
32	a	993	G
32	a	994	A
32	a	996	A
32	a	999	C
32	a	1001	C
32	a	1004	A
32	a	1009	U
32	a	1017	U
32	a	1018	G
32	a	1023	U
32	a	1024	G
32	a	1026	G
32	a	1028	C
32	a	1029	U
32	a	1030	U
32	a	1031	C
32	a	1032	G
32	a	1033	G
32	a	1034	G
32	a	1036	A
32	a	1037	C
32	a	1043	G
32	a	1044	A
32	a	1046	A
32	a	1053	G
32	a	1054	C
32	a	1056	U
32	a	1061	G
32	a	1065	U
32	a	1070	U
32	a	1081	A
32	a	1082	A
32	a	1085	U
32	a	1087	G
32	a	1088	G
32	a	1089	G
32	a	1094	G
32	a	1095	U
32	a	1100	C
32	a	1101	A
32	a	1110	A
32	a	1118	U

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Mol	Chain	Res	Type
32	a	1119	C
32	a	1123	U
32	a	1124	G
32	a	1125	U
32	a	1127	G
32	a	1132	C
32	a	1136	C
32	a	1137	C
32	a	1138	G
32	a	1139	G
32	a	1140	C
32	a	1141	C
32	a	1142	G
32	a	1143	G
32	a	1145	A
32	a	1146	A
32	a	1148	U
32	a	1150	A
32	a	1151	A
32	a	1152	A
32	a	1157	A
32	a	1159	U
32	a	1160	G
32	a	1168	U
32	a	1169	A
32	a	1171	A
32	a	1174	G
32	a	1181	G
32	a	1184	G
32	a	1190	G
32	a	1191	A
32	a	1193	G
32	a	1194	U
32	a	1195	C
32	a	1196	A
32	a	1197	A
32	a	1200	C
32	a	1201	A
32	a	1204	A
32	a	1207	2MG
32	a	1212	U
32	a	1213	A

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Mol	Chain	Res	Type
32	a	1220	G
32	a	1221	G
32	a	1224	U
32	a	1225	A
32	a	1226	C
32	a	1227	A
32	a	1229	A
32	a	1236	A
32	a	1238	A
32	a	1239	A
32	a	1240	U
32	a	1256	A
32	a	1257	A
32	a	1258	G
32	a	1260	G
32	a	1261	A
32	a	1266	G
32	a	1267	C
32	a	1271	A
32	a	1275	A
32	a	1278	G
32	a	1280	A
32	a	1281	C
32	a	1282	C
32	a	1283	U
32	a	1286	U
32	a	1287	A
32	a	1298	U
32	a	1299	A
32	a	1300	G
32	a	1302	C
32	a	1305	G
32	a	1309	G
32	a	1314	C
32	a	1317	C
32	a	1318	A
32	a	1322	C
32	a	1324	A
32	a	1327	C
32	a	1331	G
32	a	1332	A
32	a	1336	C

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Mol	Chain	Res	Type
32	a	1346	A
32	a	1347	G
32	a	1348	U
32	a	1351	U
32	a	1359	C
32	a	1361	G
32	a	1362	A
32	a	1363	A
32	a	1366	C
32	a	1370	G
32	a	1374	A
32	a	1375	A
32	a	1379	G
32	a	1381	U
32	a	1389	C
32	a	1394	A
32	a	1395	C
32	a	1397	C
32	a	1404	C
32	a	1419	G
32	a	1422	G
32	a	1427	C
32	a	1428	A
32	a	1429	A
32	a	1432	G
32	a	1433	A
32	a	1436	U
32	a	1441	A
32	a	1446	A
32	a	1448	C
32	a	1452	C
32	a	1453	G
32	a	1455	G
32	a	1458	G
32	a	1491	G
32	a	1492	A
32	a	1493	A
32	a	1494	G
32	a	1499	A
32	a	1502	A
32	a	1503	A
32	a	1506	U

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Mol	Chain	Res	Type
32	a	1517	G
32	a	1520	C
32	a	1529	G
32	a	1530	G
32	a	1533	C
32	a	1534	A
55	x	5	G
55	x	7	U
55	x	8	G
55	x	12	C
55	x	15	C
55	x	17	U
55	x	18	G
55	x	19	G
55	x	20	U
55	x	21	A
55	x	22	G
55	x	26	G
55	x	35	A
55	x	36	U
55	x	47	U
55	x	48	C
55	x	49	G
55	x	50	U
55	x	52	G
55	x	59	A
55	x	60	U
55	x	76	A
55	y	4	G
55	y	5	G
55	y	15	C
55	y	16	C
55	y	18	G
55	y	20	U
55	y	21	A
55	y	22	G
55	y	35	A
55	y	37	A
55	y	46	G
55	y	47	U
55	y	48	C
55	y	49	G

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Mol	Chain	Res	Type
55	y	55	U
55	y	60	U
55	y	61	C
55	y	76	A
56	z	45	A

All (83) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	62	U
1	A	100	U
1	A	119	A
1	A	137	U
1	A	177	G
1	A	181	A
1	A	196	A
1	A	197	A
1	A	212	G
1	A	249	C
1	A	264	C
1	A	271	G
1	A	279	A
1	A	310	A
1	A	322	A
1	A	404	A
1	A	412	A
1	A	446	G
1	A	455	C
1	A	463	G
1	A	481	G
1	A	506	G
1	A	512	G
1	A	620	G
1	A	675	A
1	A	728	G
1	A	733	G
1	A	762	U
1	A	764	A
1	A	784	G
1	A	830	G
1	A	884	U

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Mol	Chain	Res	Type
1	A	896	A
1	A	913	U
1	A	974	G
1	A	984	A
1	A	1088	A
1	A	1126	A
1	A	1140	C
1	A	1141	U
1	A	1151	A
1	A	1190	G
1	A	1200	C
1	A	1224	U
1	A	1288	G
1	A	1311	G
1	A	1320	C
1	A	1344	U
1	A	1379	U
1	A	1602	U
1	A	1608	A
1	A	1730	C
1	A	1786	A
1	A	1857	G
1	A	1884	G
1	A	1918	A
1	A	1937	A
1	A	1939	5MU
1	A	2074	U
1	A	2146	C
1	A	2157	G
1	A	2182	U
1	A	2193	G
1	A	2225	A
1	A	2286	G
1	A	2324	U
1	A	2326	C
1	A	2427	C
1	A	2458	G
1	A	2504	PSU
1	A	2517	C
1	A	2519	U
1	A	2581	G
1	A	2595	G

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Mol	Chain	Res	Type
1	A	2602	A
1	A	2638	G
1	A	2645	G
1	A	2681	C
1	A	2790	U
1	A	2808	G
1	A	2893	A
2	B	40	U

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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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. '-' 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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
1	A	1917	PSU	C6-C5	3.79	1.39	1.35
1	A	2605	PSU	C6-C5	3.74	1.39	1.35
1	A	2580	PSU	C6-C5	3.49	1.39	1.35
1	A	747	5MU	C2-N1	3.29	1.43	1.38
32	a	967	5MC	C6-C5	3.21	1.39	1.34
1	A	2504	PSU	C6-C5	3.20	1.39	1.35
32	a	1498	UR3	C2-N1	2.95	1.42	1.38
1	A	747	5MU	C4-C5	2.94	1.49	1.44
1	A	1939	5MU	C4-N3	-2.90	1.33	1.38
1	A	2605	PSU	C4-N3	-2.86	1.33	1.38
1	A	2580	PSU	C4-N3	-2.80	1.33	1.38
1	A	1962	5MC	C6-C5	2.73	1.39	1.34
1	A	747	5MU	C6-C5	2.71	1.39	1.34
1	A	1939	5MU	C6-C5	2.69	1.39	1.34
1	A	2457	PSU	C4-N3	-2.67	1.33	1.38
1	A	2552	OMU	C2-N1	2.66	1.42	1.38
32	a	1519	MA6	C5-C4	2.60	1.47	1.40
1	A	2504	PSU	C4-N3	-2.59	1.34	1.38
1	A	1835	2MG	C6-N1	-2.56	1.34	1.37
1	A	2251	OMG	C6-N1	-2.51	1.34	1.37
1	A	1939	5MU	C2-N1	2.48	1.42	1.38
32	a	1518	MA6	C5-C4	2.43	1.47	1.40
32	a	1407	5MC	C6-C5	2.43	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	747	5MU	C4-N3	-2.41	1.34	1.38
1	A	1911	PSU	C4-N3	-2.36	1.34	1.38
1	A	746	PSU	C4-N3	-2.31	1.34	1.38
1	A	955	PSU	C4-N3	-2.24	1.34	1.38
1	A	2552	OMU	C4-N3	-2.23	1.34	1.38
32	a	1519	MA6	C6-N1	2.20	1.36	1.33
1	A	1917	PSU	C4-N3	-2.18	1.34	1.38
1	A	2251	OMG	O4'-C1'	2.16	1.44	1.41
1	A	1939	5MU	C2-N3	-2.16	1.34	1.38
1	A	2552	OMU	C6-C5	2.14	1.40	1.35
32	a	516	PSU	C4-C5	2.11	1.50	1.44
32	a	1518	MA6	C6-N1	2.11	1.36	1.33
1	A	955	PSU	C4-C5	2.11	1.50	1.44
1	A	1939	5MU	C6-N1	-2.10	1.34	1.38
1	A	2580	PSU	C2-N3	-2.07	1.34	1.37
1	A	2498	OMC	C6-C5	2.05	1.39	1.35
32	a	1516	2MG	C6-N1	-2.05	1.34	1.37
32	a	516	PSU	C4-N3	-2.05	1.35	1.38
1	A	2457	PSU	C4-C5	2.05	1.50	1.44
1	A	1917	PSU	C4-C5	2.04	1.50	1.44

All (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
1	A	2504	PSU	N1-C2-N3	5.99	121.91	115.13
1	A	746	PSU	N1-C2-N3	5.98	121.91	115.13
1	A	955	PSU	N1-C2-N3	5.91	121.83	115.13
32	a	516	PSU	N1-C2-N3	5.58	121.45	115.13
1	A	1917	PSU	N1-C2-N3	5.46	121.32	115.13
1	A	1911	PSU	N1-C2-N3	5.45	121.31	115.13
1	A	747	5MU	N3-C2-N1	5.04	121.58	114.89
1	A	1939	5MU	N3-C2-N1	4.79	121.25	114.89
1	A	1939	5MU	C4-N3-C2	-4.65	121.33	127.35
1	A	747	5MU	C4-N3-C2	-4.59	121.41	127.35
1	A	2552	OMU	N3-C2-N1	4.59	120.98	114.89
1	A	2605	PSU	C4-N3-C2	-4.53	119.81	126.34
1	A	2552	OMU	C4-N3-C2	-4.18	121.06	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	746	PSU	C4-N3-C2	-3.98	120.61	126.34
1	A	2504	PSU	C4-N3-C2	-3.95	120.64	126.34
1	A	1939	5MU	C5-C4-N3	3.89	118.64	115.31
1	A	2580	PSU	C4-N3-C2	-3.85	120.79	126.34
1	A	2504	PSU	C3'-C2'-C1'	3.83	106.10	101.64
1	A	955	PSU	C4-N3-C2	-3.79	120.88	126.34
32	a	1519	MA6	C4-C5-N7	-3.77	105.47	109.40
1	A	2457	PSU	C4-N3-C2	-3.75	120.94	126.34
1	A	1911	PSU	C4-N3-C2	-3.74	120.95	126.34
1	A	1939	5MU	C5-C6-N1	-3.73	119.50	123.34
32	a	516	PSU	C4-N3-C2	-3.62	121.12	126.34
1	A	747	5MU	C5-C4-N3	3.62	118.40	115.31
1	A	955	PSU	O2-C2-N1	-3.58	118.84	122.79
1	A	1917	PSU	O2-C2-N1	-3.57	118.86	122.79
1	A	1917	PSU	C4-N3-C2	-3.50	121.30	126.34
1	A	747	5MU	C5M-C5-C4	3.48	122.59	118.77
1	A	2504	PSU	O2-C2-N1	-3.41	119.04	122.79
1	A	746	PSU	O2-C2-N1	-3.39	119.05	122.79
1	A	2457	PSU	O2-C2-N1	-3.33	119.12	122.79
32	a	1518	MA6	N3-C2-N1	-3.30	123.52	128.68
1	A	1911	PSU	O2-C2-N1	-3.30	119.16	122.79
1	A	2552	OMU	C5-C4-N3	3.29	119.76	114.84
32	a	516	PSU	O2-C2-N1	-3.27	119.19	122.79
1	A	1962	5MC	O2-C2-N3	-3.25	117.04	122.33
32	a	966	2MG	C3'-C2'-C1'	3.24	105.86	100.98
32	a	1519	MA6	N3-C2-N1	-3.23	123.62	128.68
1	A	2605	PSU	O2-C2-N1	-3.21	119.26	122.79
32	a	1519	MA6	N1-C6-N6	3.16	120.38	117.06
32	a	1519	MA6	C10-N6-C9	-3.15	105.97	116.12
32	a	967	5MC	O2-C2-N3	-3.14	117.22	122.33
1	A	1939	5MU	O4-C4-C5	-3.13	121.27	124.90
32	a	516	PSU	C3'-C2'-C1'	3.10	105.24	101.64
1	A	745	1MG	O6-C6-C5	-3.06	118.78	124.19
32	a	1407	5MC	O2-C2-N3	-3.02	117.42	122.33
1	A	747	5MU	C5M-C5-C6	-3.02	118.82	122.85
1	A	1917	PSU	C3'-C2'-C1'	2.98	105.11	101.64
1	A	1917	PSU	C6-C5-C4	-2.93	116.15	118.20
1	A	2580	PSU	O2-C2-N1	-2.93	119.57	122.79
1	A	2457	PSU	C3'-C2'-C1'	2.92	105.04	101.64
1	A	2498	OMC	O2-C2-N3	-2.90	117.61	122.33
32	a	967	5MC	C5-C4-N3	-2.90	118.54	121.67
32	a	1407	5MC	C5-C6-N1	-2.87	120.38	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2552	OMU	O4-C4-C5	-2.87	120.12	125.16
32	a	1518	MA6	C3'-C2'-C1'	2.86	105.28	100.98
1	A	1962	5MC	C5-C4-N3	-2.82	118.63	121.67
1	A	1835	2MG	C5-C6-N1	2.77	118.85	113.95
1	A	1962	5MC	CM5-C5-C6	-2.74	119.19	122.85
1	A	2580	PSU	C3'-C2'-C1'	2.73	104.82	101.64
32	a	1402	4OC	O2-C2-N3	-2.69	117.95	122.33
1	A	1911	PSU	C6-C5-C4	-2.64	116.35	118.20
32	a	1407	5MC	CM5-C5-C6	-2.63	119.34	122.85
1	A	2251	OMG	C5-C6-N1	2.60	118.54	113.95
32	a	1519	MA6	C9-N6-C6	-2.58	111.69	119.51
32	a	1407	5MC	C5-C4-N3	-2.55	118.92	121.67
32	a	1519	MA6	C10-N6-C6	-2.54	111.83	119.51
1	A	747	5MU	O4-C4-C5	-2.53	121.97	124.90
1	A	745	1MG	C5-C6-N1	2.52	117.70	113.90
32	a	1518	MA6	C9-N6-C6	-2.52	111.90	119.51
32	a	966	2MG	C5-C6-N1	2.48	118.33	113.95
1	A	747	5MU	O2-C2-N3	-2.46	116.91	121.50
1	A	747	5MU	C1'-N1-C2	2.46	122.02	117.57
1	A	1939	5MU	O4'-C1'-N1	2.45	113.97	108.36
1	A	1962	5MC	C5-C6-N1	-2.44	120.83	123.34
1	A	2445	2MG	C5-C6-N1	2.42	118.23	113.95
1	A	747	5MU	C5-C6-N1	-2.42	120.85	123.34
32	a	1207	2MG	C5-C6-N1	2.40	118.19	113.95
32	a	516	PSU	C6-C5-C4	-2.38	116.54	118.20
1	A	2552	OMU	C6-N1-C2	-2.38	117.95	120.99
32	a	1516	2MG	C5-C6-N1	2.37	118.14	113.95
32	a	1402	4OC	C6-C5-C4	2.35	119.84	116.96
1	A	745	1MG	CM1-N1-C6	2.32	120.72	117.55
1	A	2580	PSU	O4'-C1'-C2'	2.28	108.36	105.14
1	A	747	5MU	C3'-C2'-C1'	2.26	105.72	101.43
32	a	1207	2MG	C8-N7-C5	2.25	107.28	102.99
32	a	1402	4OC	O4'-C1'-N1	2.23	113.47	108.36
32	a	1207	2MG	C3'-C2'-C1'	2.22	104.33	100.98
1	A	745	1MG	C8-N7-C5	2.21	107.20	102.99
1	A	1939	5MU	O2-C2-N3	-2.21	117.39	121.50
1	A	2445	2MG	O6-C6-C5	-2.20	120.07	124.37
32	a	1516	2MG	C8-N7-C5	2.19	107.16	102.99
1	A	2498	OMC	O4'-C1'-N1	2.19	113.36	108.36
32	a	967	5MC	CM5-C5-C6	-2.19	119.93	122.85
32	a	1402	4OC	C5-C4-N4	-2.16	118.21	122.61
1	A	2605	PSU	C5-C6-N1	-2.15	118.89	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	967	5MC	C3'-C2'-C1'	2.11	105.44	101.43
32	a	1518	MA6	C4-C5-N7	-2.11	107.20	109.40
32	a	967	5MC	C5-C6-N1	-2.10	121.18	123.34
1	A	1835	2MG	C8-N7-C5	2.10	106.99	102.99
1	A	747	5MU	C6-N1-C2	-2.10	119.17	121.30
1	A	2445	2MG	C8-N7-C5	2.06	106.91	102.99
32	a	1498	UR3	O3'-C3'-C4'	2.05	116.98	111.05
1	A	2498	OMC	C1'-N1-C2	2.05	123.00	118.42
32	a	1498	UR3	C3'-C2'-C1'	2.05	105.31	101.43
32	a	1519	MA6	C3'-C2'-C1'	2.04	104.04	100.98
1	A	2251	OMG	C8-N7-C5	2.04	106.87	102.99
32	a	1498	UR3	C3U-N3-C4	2.02	120.78	117.89
1	A	2552	OMU	O2-C2-N3	-2.01	117.75	121.50
32	a	1498	UR3	C1'-N1-C2	2.01	120.39	116.99
32	a	967	5MC	O4'-C1'-N1	2.01	112.96	108.36
32	a	1518	MA6	C10-N6-C9	-2.01	109.64	116.12
1	A	2504	PSU	O4'-C1'-C2'	2.01	107.98	105.14
1	A	2504	PSU	C5-C6-N1	-2.00	119.10	122.11

There are no chirality outliers.

All (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
53	v	252	MEQ	C-CA-CB-CG
1	A	746	PSU	C3'-C4'-C5'-O5'
1	A	1939	5MU	C3'-C4'-C5'-O5'
1	A	1939	5MU	O4'-C4'-C5'-O5'
1	A	2457	PSU	O4'-C4'-C5'-O5'
32	a	966	2MG	C3'-C4'-C5'-O5'
32	a	1402	4OC	C3'-C4'-C5'-O5'
32	a	1518	MA6	O4'-C4'-C5'-O5'
32	a	1519	MA6	O4'-C4'-C5'-O5'
1	A	1835	2MG	C3'-C4'-C5'-O5'
1	A	2445	2MG	O4'-C4'-C5'-O5'
1	A	2457	PSU	C3'-C4'-C5'-O5'
32	a	966	2MG	O4'-C4'-C5'-O5'
32	a	1518	MA6	C3'-C4'-C5'-O5'
32	a	1519	MA6	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1835	2MG	O4'-C4'-C5'-O5'
32	a	1207	2MG	C3'-C4'-C5'-O5'
32	a	1207	2MG	O4'-C4'-C5'-O5'
32	a	1207	2MG	C4'-C5'-O5'-P
32	a	1519	MA6	C5-C6-N6-C9
32	a	1519	MA6	C4'-C5'-O5'-P
1	A	746	PSU	O4'-C1'-C5-C4
1	A	2498	OMC	C2'-C1'-N1-C2
32	a	1518	MA6	N1-C6-N6-C9

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.

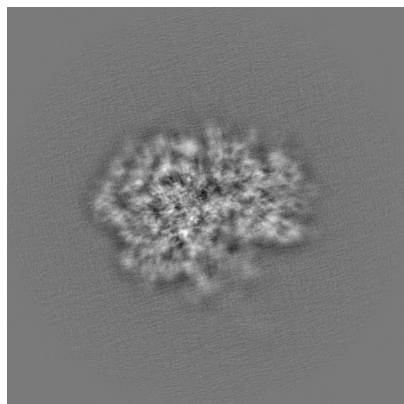
6 Map visualisation [i](#)

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.

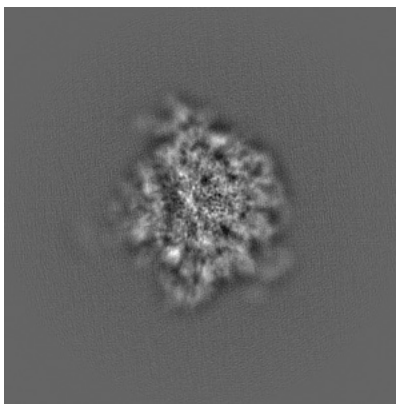
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

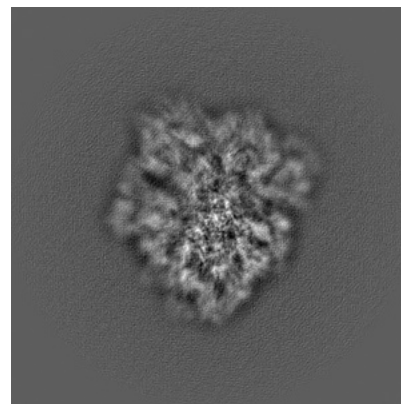
6.1.1 Primary map



X

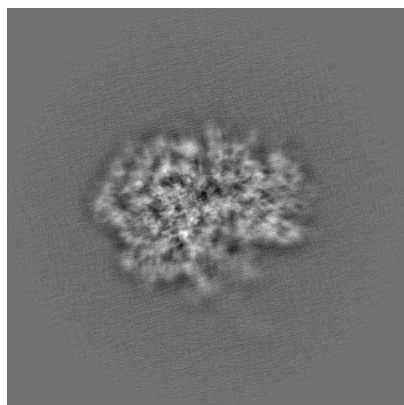


Y

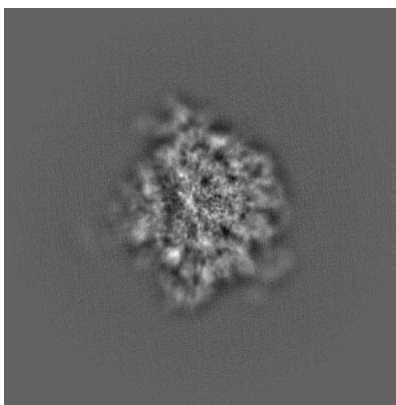


Z

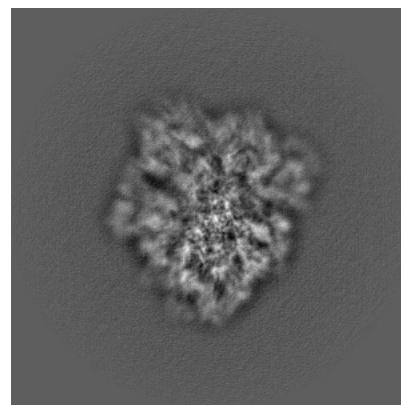
6.1.2 Raw map



X



Y

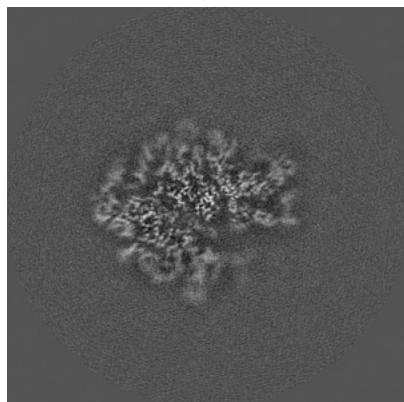


Z

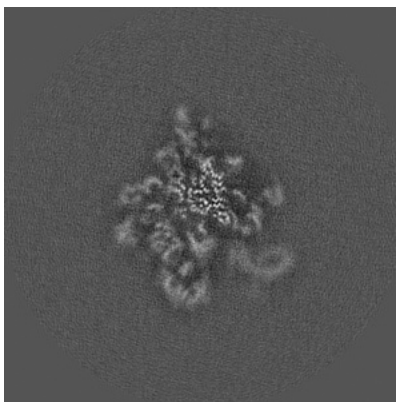
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

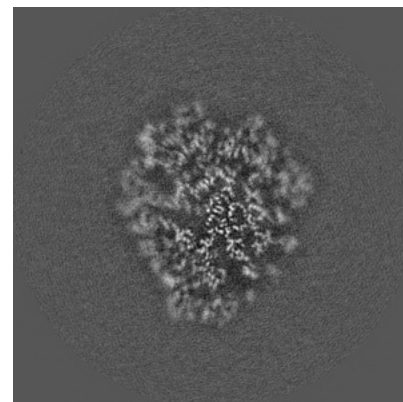
6.2.1 Primary map



X Index: 192

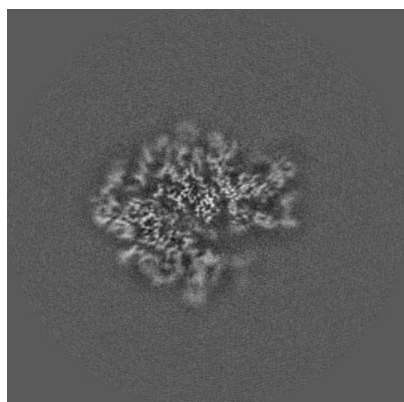


Y Index: 192

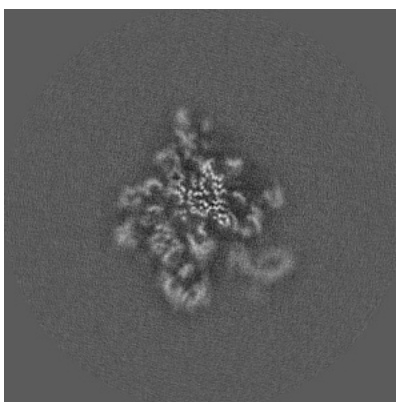


Z Index: 192

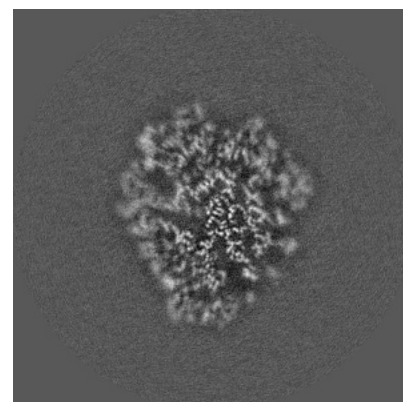
6.2.2 Raw map



X Index: 192



Y Index: 192

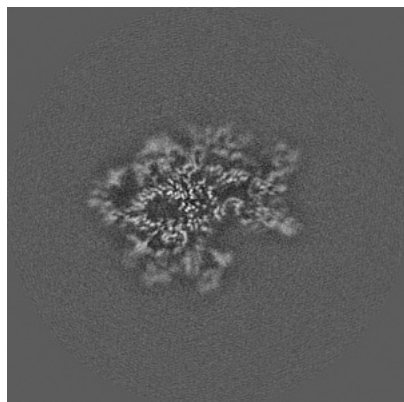


Z Index: 192

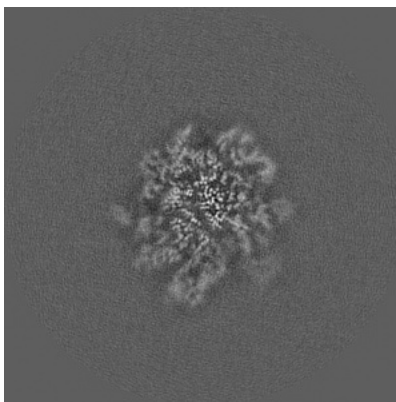
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

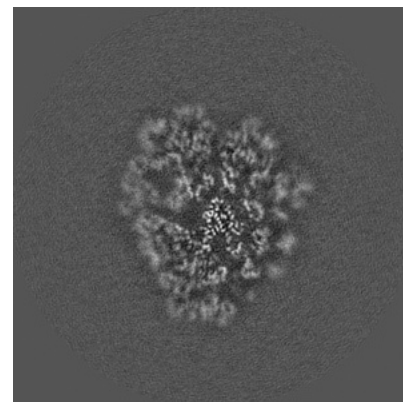
6.3.1 Primary map



X Index: 201

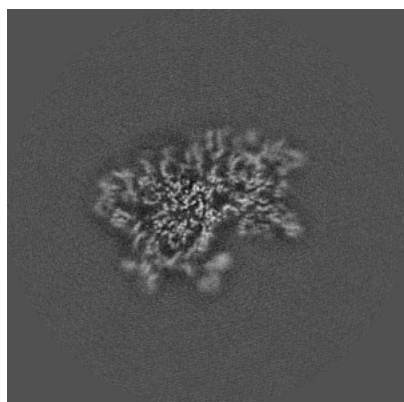


Y Index: 170

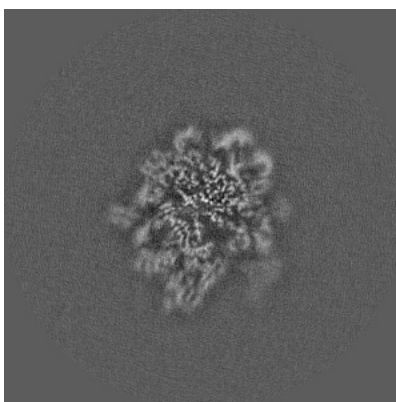


Z Index: 195

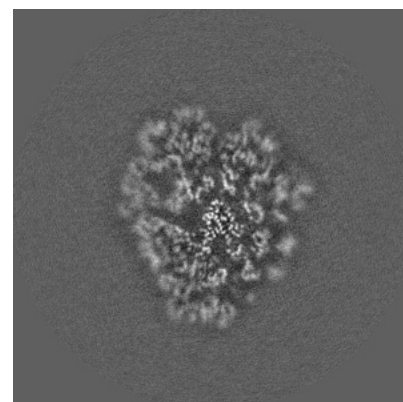
6.3.2 Raw map



X Index: 207



Y Index: 174

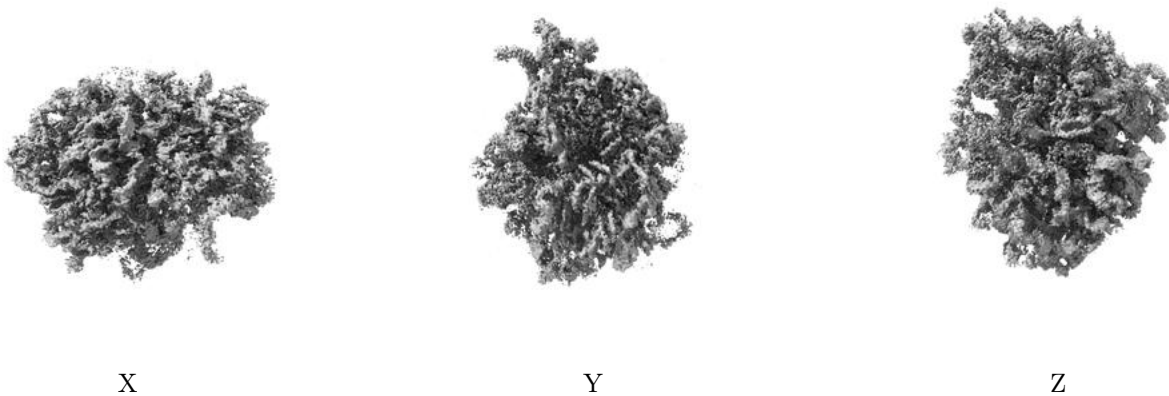


Z Index: 195

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

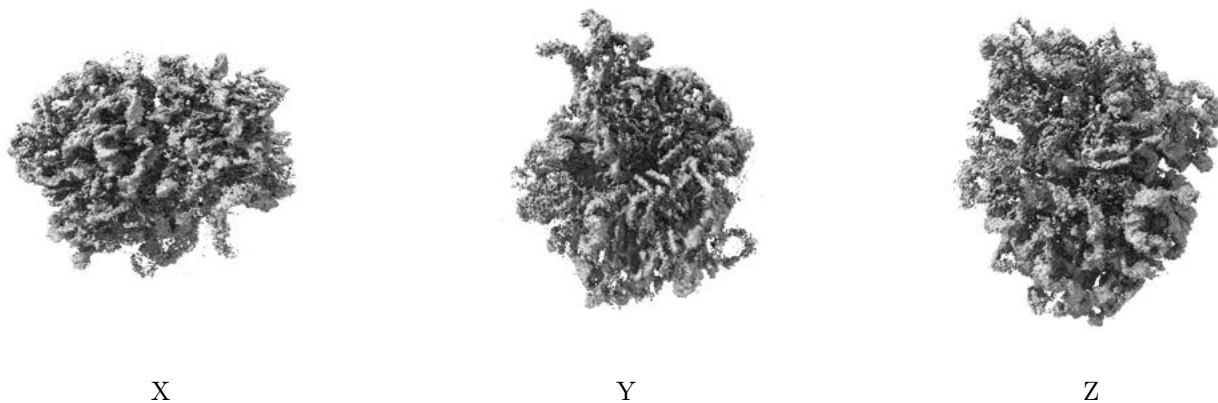
6.4 Orthogonal surface views [i](#)

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.

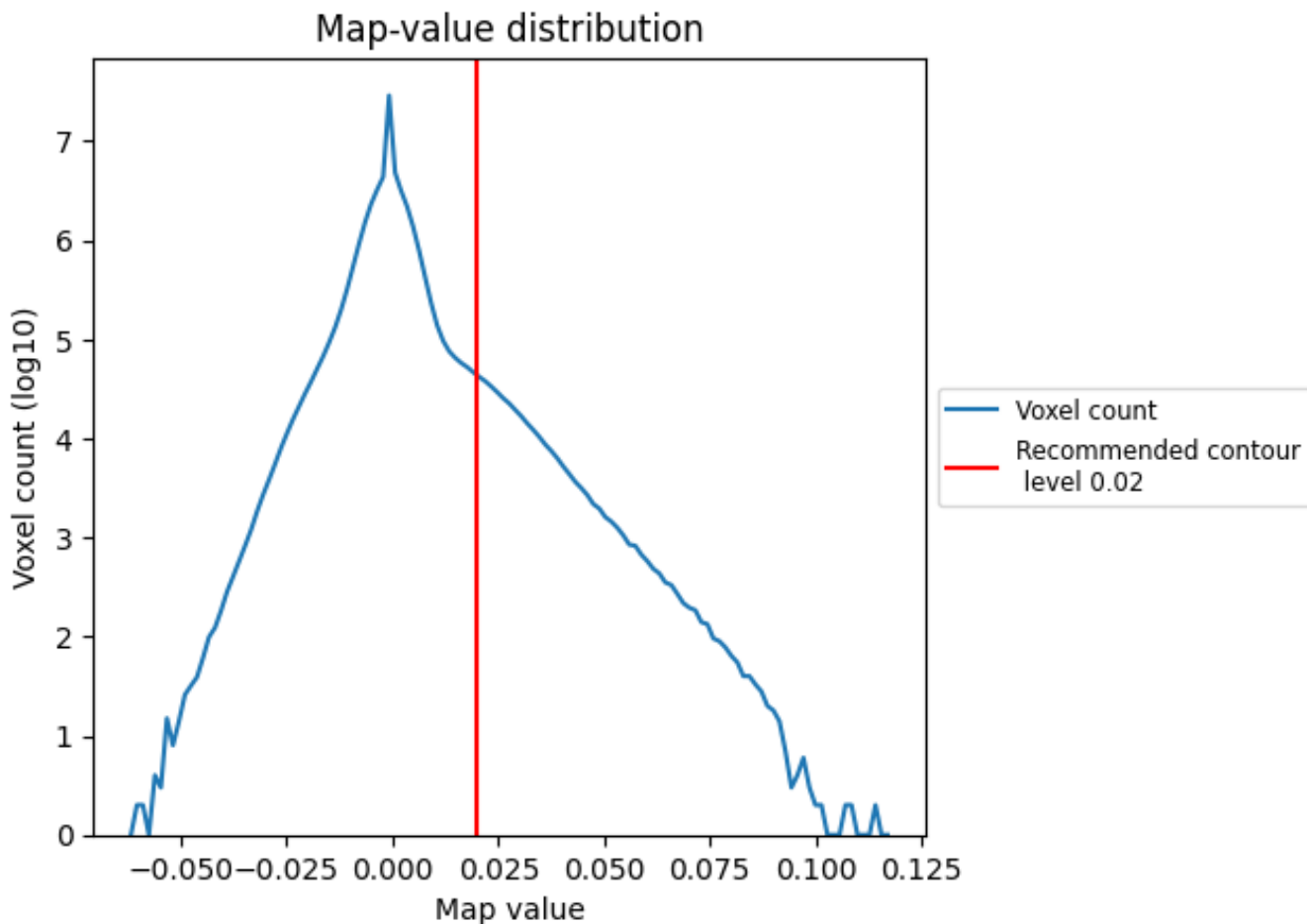
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

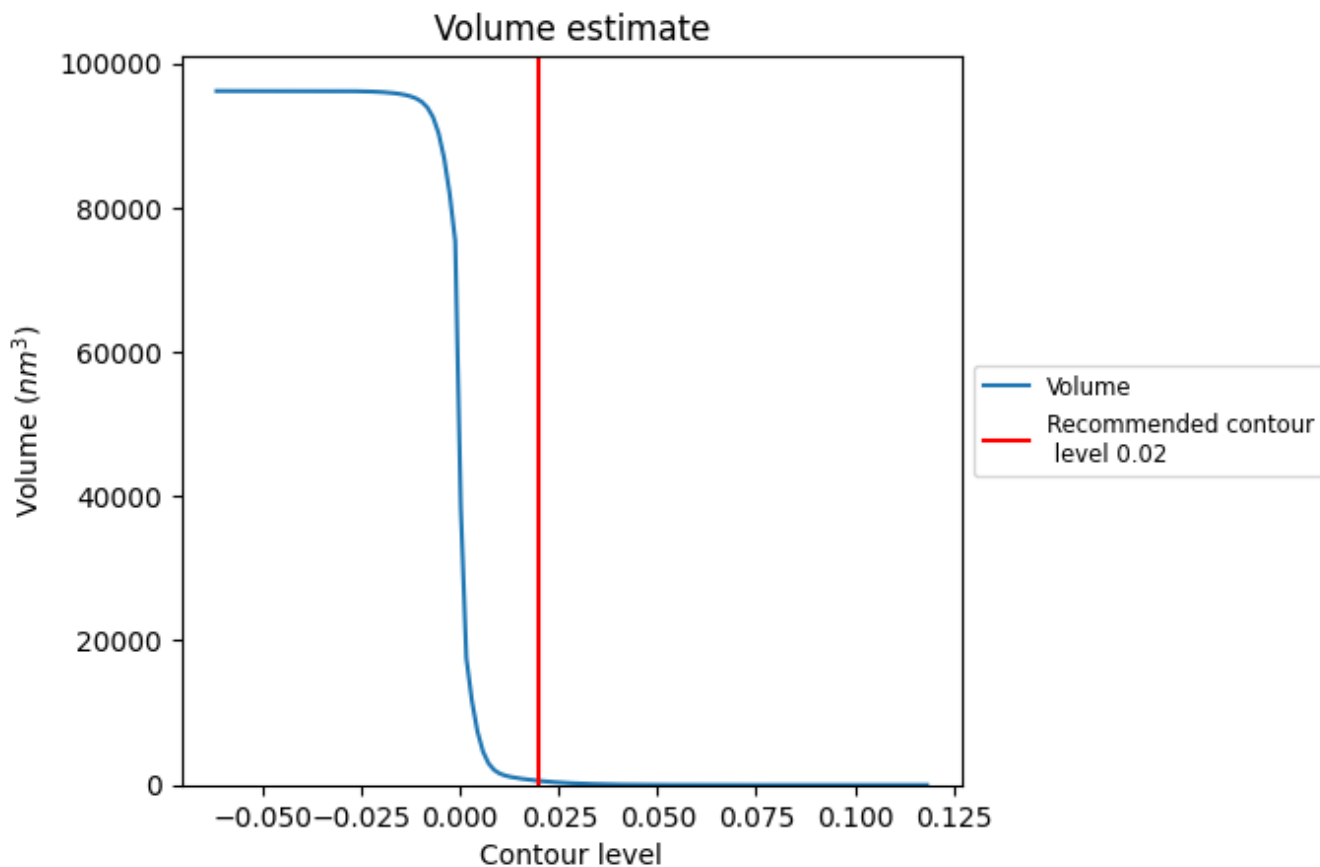
This section contains the results of statistical analysis of the map.

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.

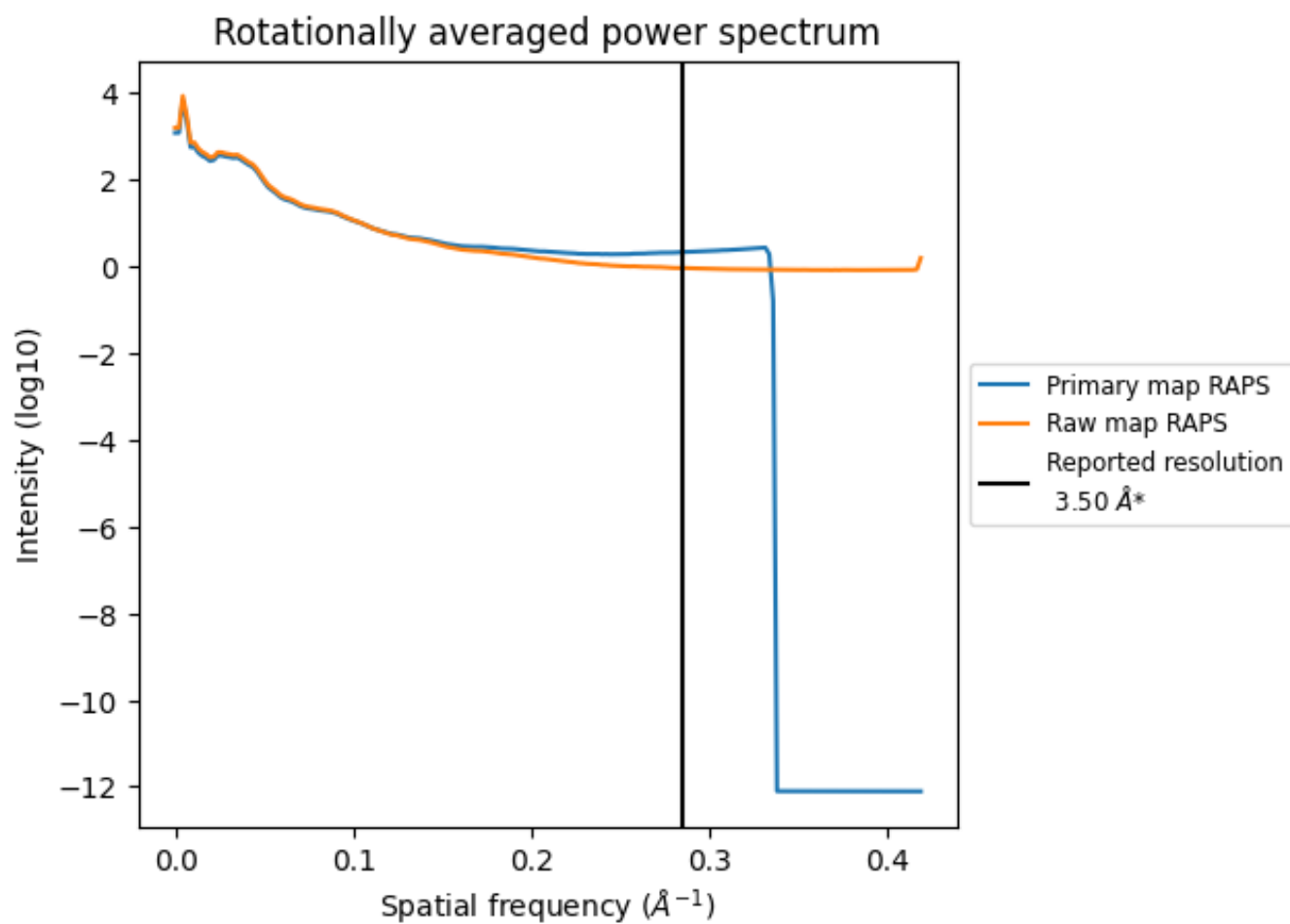
7.2 Volume estimate [i](#)



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](#)

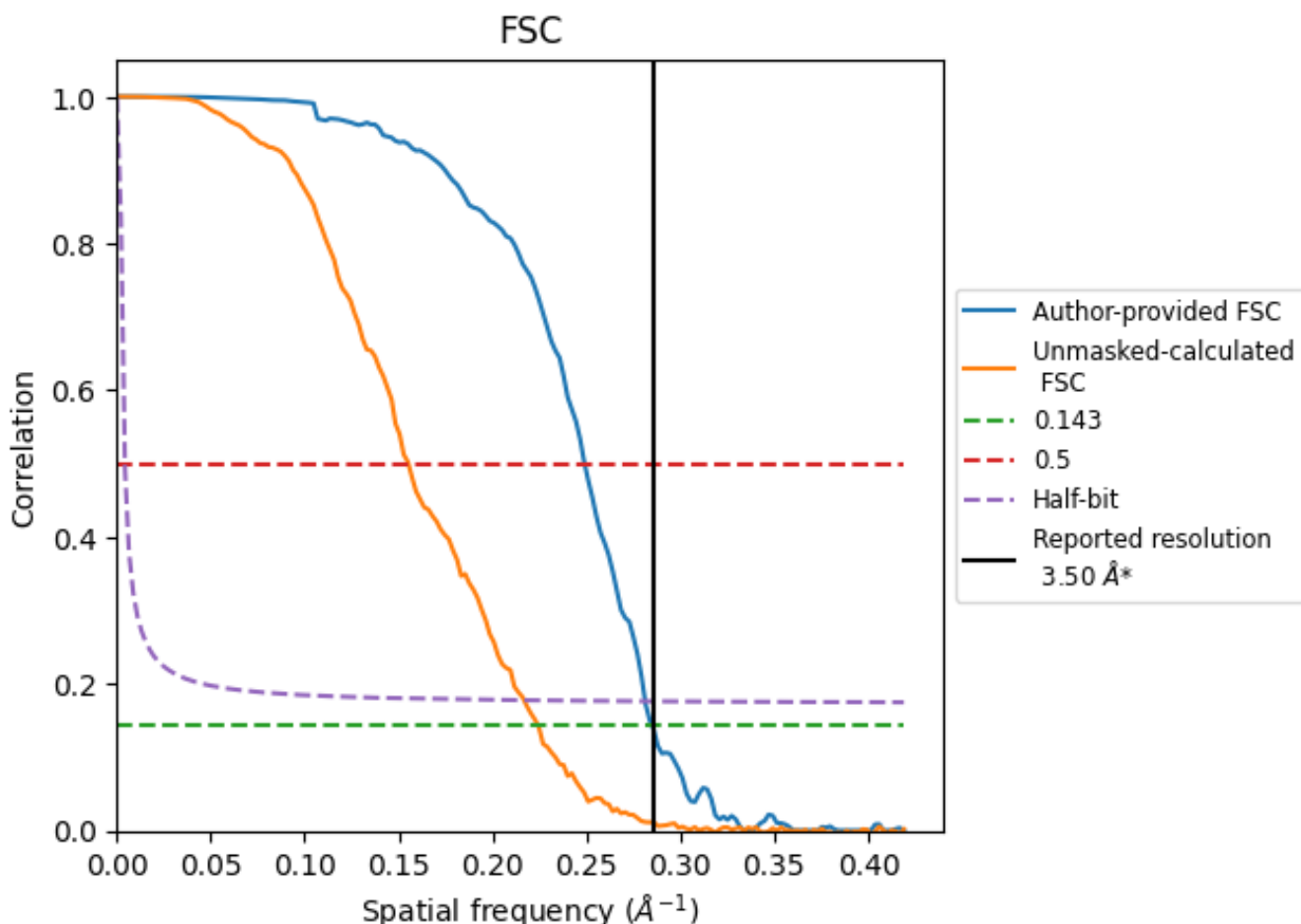


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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](#)

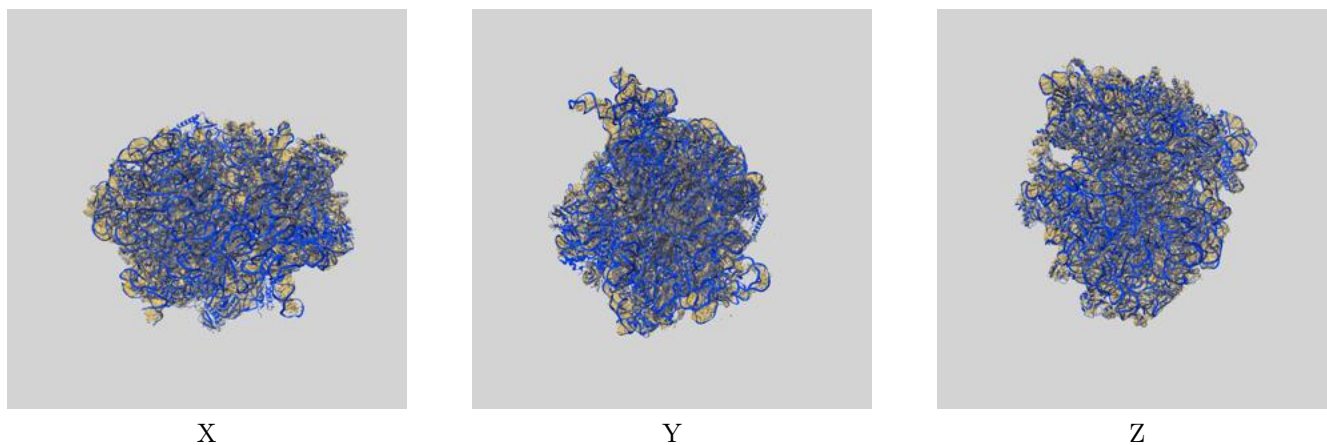
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	4.01	3.55
Unmasked-calculated*	4.46	6.44	4.61

*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](#)

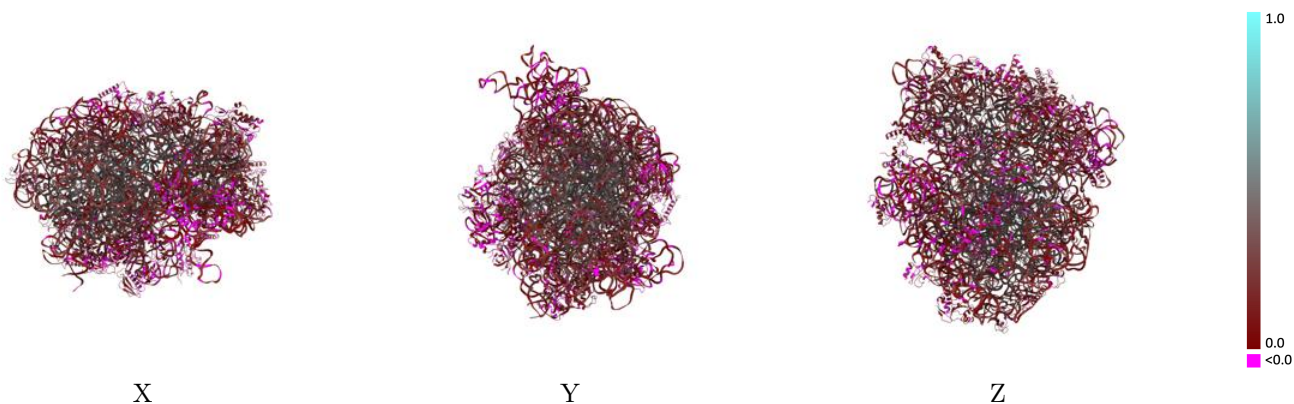
This section contains information regarding the fit between EMDB map EMD-8505 and PDB model 5U4I. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



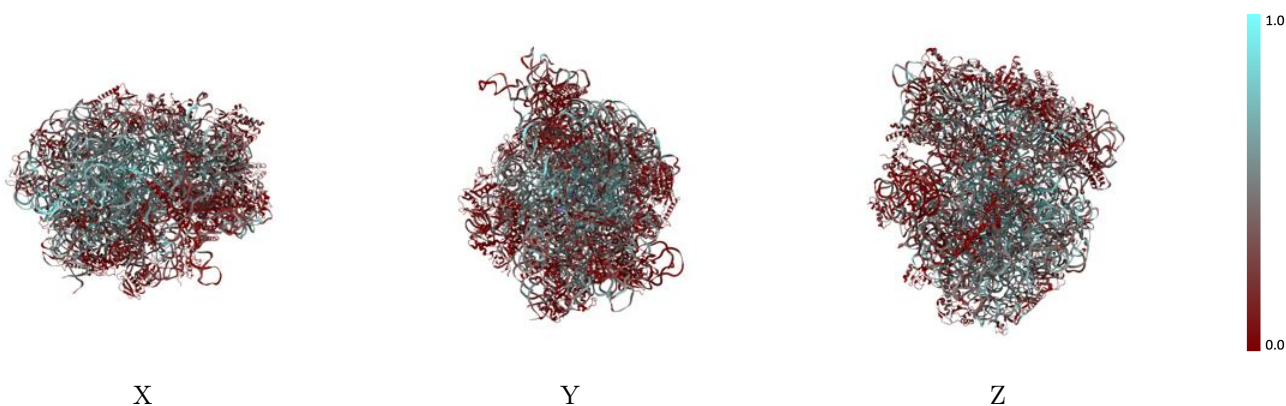
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



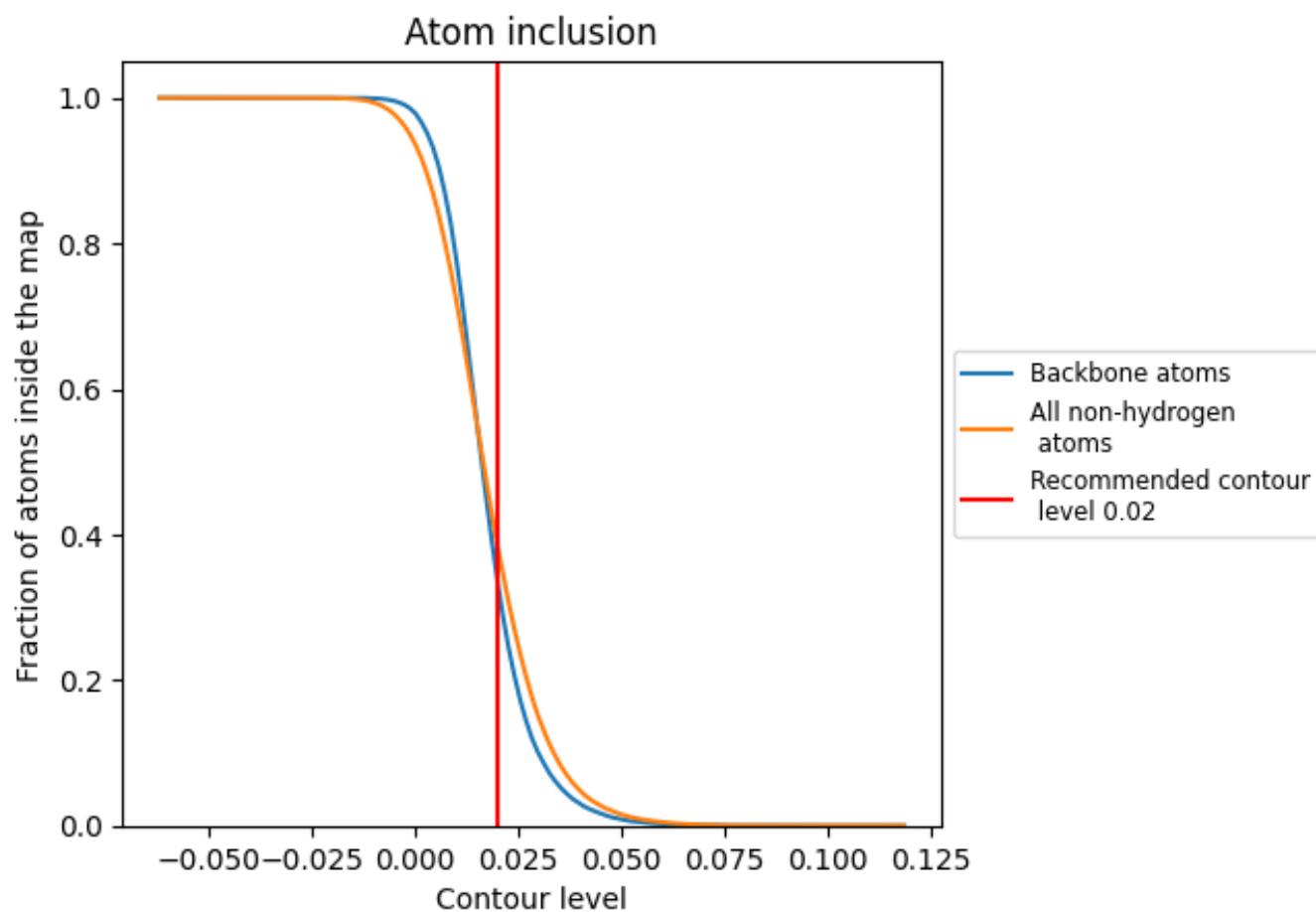
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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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