

SUPPLEMENTARY MATERIAL

The adenosine wedge: a new structural motif in ribosomal RNA

Matthieu G. Gagnon and Sergey V. Steinberg*

Département de Biochimie, Université de Montréal, Montréal, Québec H3C 3J7, Canada

*Corresponding author. Département de Biochimie, Université de Montréal, C.P. 6128, Succursale Centre-Ville, Montréal, Québec H3C 3J7, Canada. Tel. : +1 514 343 6320; Fax : +1 514 343 2210; E-mail : serguei.chteinberg@umontreal.ca

SUPPLEMENTAL TABLES

Supplemental Table 1. List of hydrogen bonds formed in the adenosine wedge motif

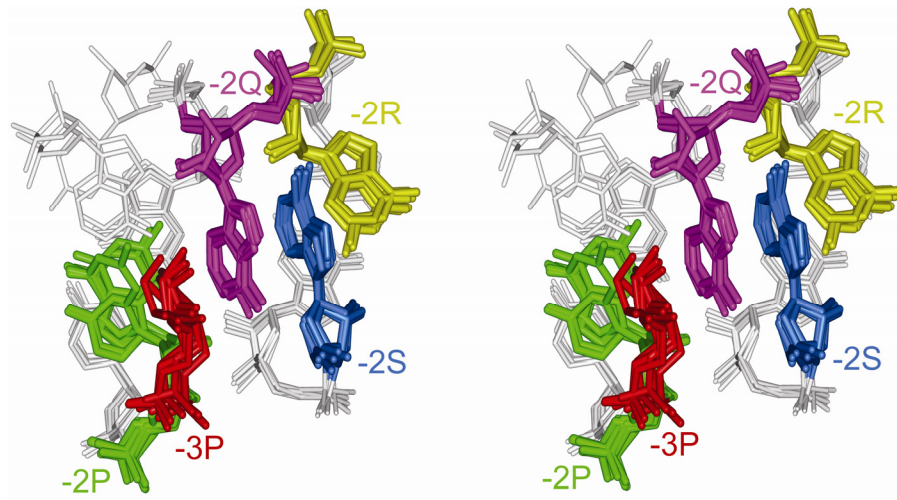
Hydrogen bonds	Symmetric / Asymmetric	Comments
N6 (-2S) – O5' (-2Q)	Asymmetric	Requires that -2R and -2Q be covalently connected (not shown)
N1 (-2Q) – O2' (-2P)	Symmetric	A-minor interaction between -2Q and -2P (Fig. 3A-E) and between -2S and -2R (Fig. 3F-H)
N1 (-2S) – O2' (-2R)		
N2 (-2R if G) – O2' (-2S)	Asymmetric	Is possible due to the displacement of the A-wedge [-2Q;-2S] in direction of strand R (Fig. 3F). The symmetrical H-bond N2 (-2P if G) – O2' (-2Q) cannot be formed
N2 (-2P if G) – N3 (-2Q) / N6 (A397 in S549) – N3 (-2Q)	Symmetric	Is shown in Figure 3A, C, D and in Figure 3F
N2 (-2R if G) – N3 (-2S)		
N6 (-2Q) – O4' (-2S)	Symmetric	Is possible due to the symmetrical position of both adenosines -2Q and -2S (not shown)
N6 (-2S) – O4' (-2Q)		
N7 (A397 in S549) – O2' (-2Q)	Equivalent H-bonds	Is possible due to the proximity of A397 (Fig. 3C) and C729 (Fig. 3D) to the ribose of -2Q (G729 in Fig. 3E)
O2 (C729) – O2' (-2Q) (L639 in archaea)		
O2' (C729) – O2' (-2Q) (L639 in archaea)	No analog	Is possible due to the closeness of the position of the riboses of the two interacting nucleotides (Fig. 3D, E)

Supplemental Table 2. Statistical data on the identities of nucleotides -2P, -2R, -2Q and -2S in motifs S549, L639 and L657

AGPMs	Nucleotide position	Nucleotide identity	Number of sequences	% of total
S549	-2P	G	17	0.18
		A	7	0.07
		U	9 558	99.49
		C	25	0.26
	-2Q	A	9 506	98.95
	-2R	G	3 235	33.67
		A	4 895	50.95
		U	1 440	14.99
		C	37	0.39
	-2S	A	9 595	99.88
	397	G	6	0.06
		A	9 590	99.82
		U	3	0.03
		C	8	0.08
	TOTAL: 9 607			100
L639	-2P	G	396	92.52
		A	2	0.47
		U	2	0.47
		C	28	6.54
	-2Q	A	427	99.77
	-2R	G	381	89.02
		A	33	7.71
		U	14	3.27
		C	0	0
	-2S	A	428	100
	TOTAL: 428			100
L657	-2P	G	401	93.91
		A	26	6.09
		U	0	0
		C	0	0
	-2Q	A	426	99.77
	-2R	G	155	36.30
		A	270	63.23
		U	1	0.23
		C	1	0.23
	-2S	A	424	99.30
	TOTAL: 427			100

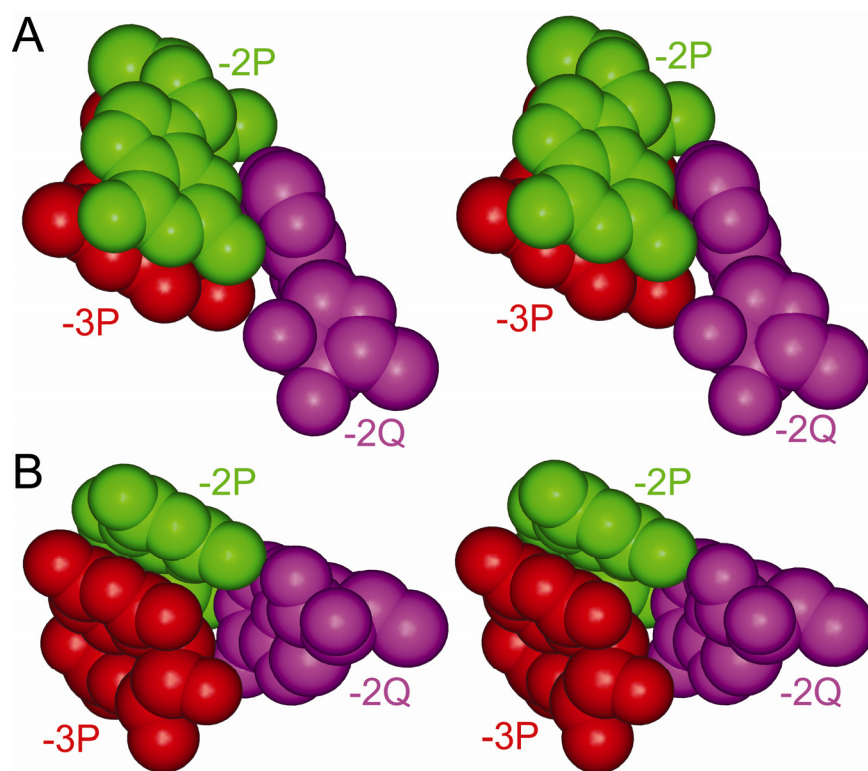
The data were obtained from the analysis of the available prokaryotic rRNA sequence alignments of the 16S and 23S rRNAs (Wuyts et al. 2004).

SUPPLEMENTAL FIGURES



Supplemental Figure 1

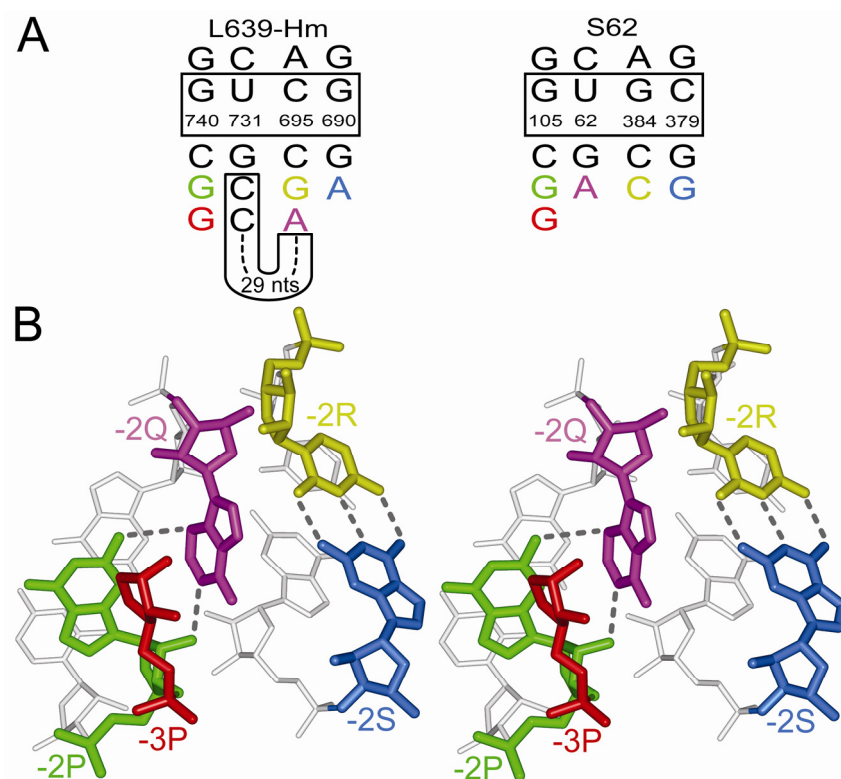
Stereo view of the superposition of seven available A-wedge motifs from three available high-resolution ribosome structures (Ban et al. 2000; Schuwirth et al. 2005; Selmer et al. 2006). The motifs are superposed based on the positions of the C1' atoms of nucleotides -2P, -3P, -2Q and -2S (r.m.s.d. = 0.36 Å). For nucleotide -3P, only the backbone and the ribose are shown. The nucleotides are colored as in Figure 2C.



Supplemental Figure 2

The space-filling representation of the [-3P;-2Q;-2P] triangle.

(A-B): Two stereo views of all three nucleotides involved in tight pair-wise interactions: two consecutive nucleotides -2P (green) and -3P (red) stack to each other. Adenosine -2Q (magenta) forms A-minor interaction with -2P and stacks to the ribose of -3P.



Supplemental Figure 3

Variations of the structure of the A-wedge motif.

(A) The nucleotide sequences of two modifications of the A-wedge motif, L639 from the *H. marismortui* 23S rRNA (L639-Hm) (Ban et al. 2000) and S62 from the *E. coli* 16S rRNA (Schuwirth et al. 2005). Each secondary structure is drawn using the same template as in Figure 2A. In each case, the nucleotide numbering is taken from the publication of the corresponding structure.

(B) Stereo view of the tertiary structure of the “half-wedge” existing in AGPM S62 from *E. coli*. The structure is oriented as in Supplemental Figure 1. The positions of nucleotides -2P, -3P and -2Q in S62 are superposable with those in the standard A-wedge arrangement with r.m.s.d. 0.59 Å, (not shown). Unlike in the standard A-wedge structure, nucleotide -2S (blue) does not stack to -2Q (magenta). Instead, it forms a WC base pair with nucleotide -2R (yellow). The nucleotide sequence and the color-code are the same as in panel A.

SUPPLEMENTAL REFERENCES

- Ban N, Nissen P, Hansen J, Moore PB, Steitz TA. 2000. The complete atomic structure of the large ribosomal subunit at 2.4 Å resolution. *Science* **289**: 905-920.
- Schuwirth BS, Borovinskaya MA, Hau CW, Zhang W, Vila-Sanjurjo A, Holton JM, Cate JH. 2005. Structures of the bacterial ribosome at 3.5 Å resolution. *Science* **310**: 827-834.
- Selmer M, Dunham CM, Murphy FV, Weixlbaumer A, Petry S, Kelley AC, Weir JR, Ramakrishnan V. 2006. Structure of the 70S ribosome complexed with mRNA and tRNA. *Science* **313**: 1935-1942.
- Wuyts J, Perriere G, Van De Peer Y. 2004. The European ribosomal RNA database. *Nucleic Acids Res.* **32**: D101-103.