Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Contribution of Dihydrouridine in Folding of the D-arm in tRNA.

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NMR data:

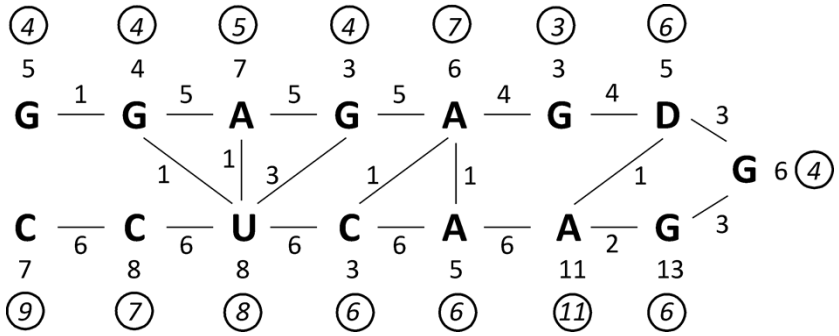

Figure S1. Schematic representation of the number of NOE distance restraints used in the structure calculations of the modified hairpin grouped as intra- and inter-nucleotide distances.

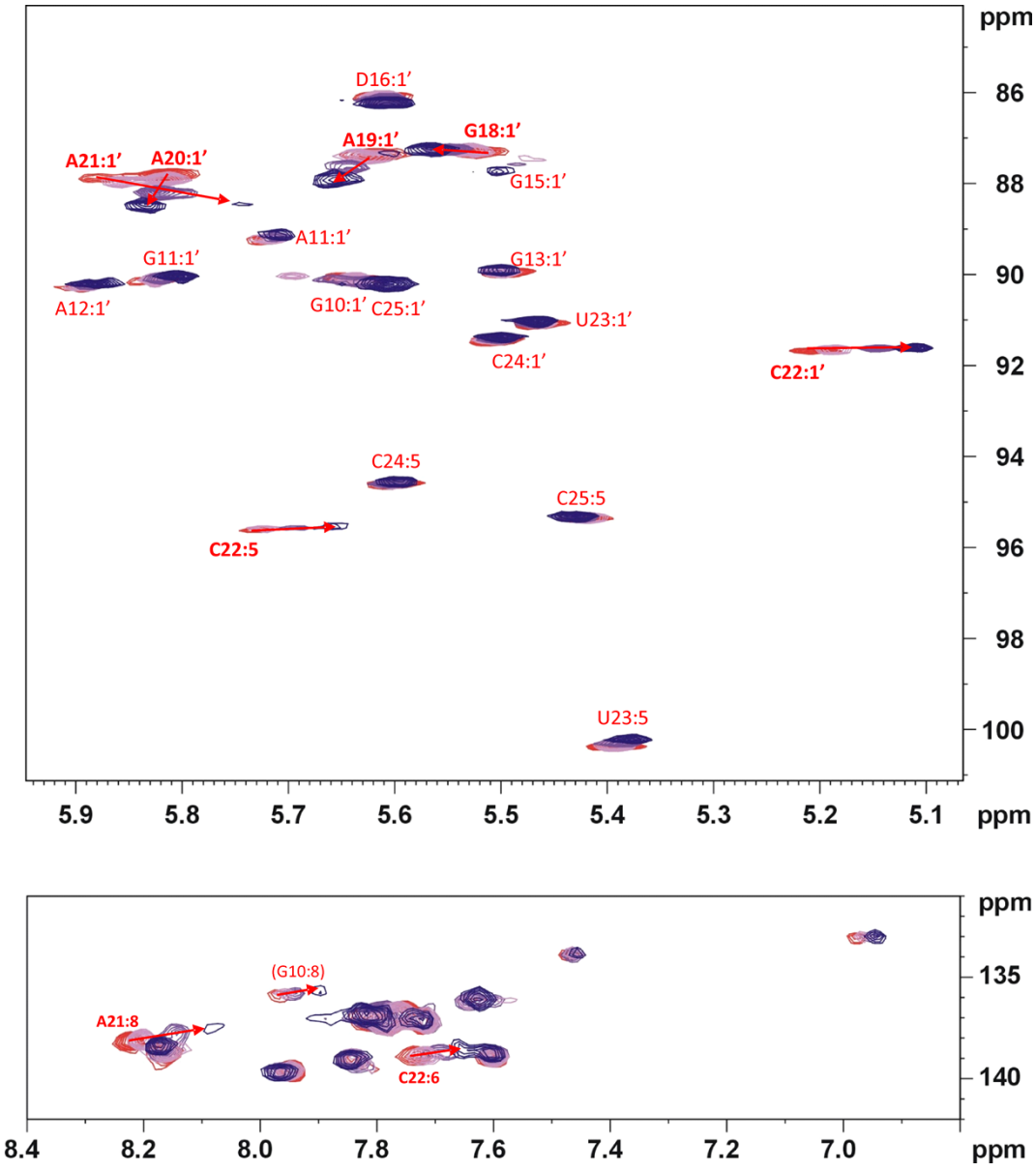

Figure S2. ^{1}H and ^{13}C chemical shift changes in the anomeric and aromatic regions of the modified D-arm at increasing [Mg^{2+}].

Molecular modelling statistics:

Table S1. NMR-based molecular modelling statistics for the 10 refined structures of the modified D-loop.

Averaged total energy (kcal.mol^{-1})	-66164 +/- 1211
Distances	284
Intra-residual NOE	87
Inter-residual NOE	186
Hydrogen bonds	11
Dihedral angles	54
Backbone	27
Ring pucker	27
Restraints violations	
NOE (>5.0 Å)	0
Angles (> 5°)	0
RMS deviation	
For NOE restraints (Å)	0.051 +/- 0.002
For dihedral restraints (°)	0.080 +/- 0.080
RMSD from mean structure (heavy atoms)	1.0 +/-0.3

Backbone torsion angles for the modified hairpin:

Table S2. Backbone torsion angles for the modified hairpin. [a]

Residue	α	β	γ	δ	ε	ζ
G1			60 (2)	89 (2)	216 (6)	295 (4)
G2	288 (5)	160 (4)	70 (2)	88 (1)	205 (8)	273 (4)
A3	277 (3)	174 (9)	67 (3)	87 (1)	205 (6)	298 (4)
G4	286 (4)	185 (6)	58 (2)	87 (2)	189 (7)	230 (98)
A5	156 (26)	172 (52)	180 (4)	93 (2)	226 (28)	268 (70)
G6	213 (77)	174 (52)	118 (57)	92 (2)	187 (7)	190 (108)
D7	171 (23)	156 (65)	176 (6)	146 (2)	204 (12)	163 (73)
G8	139 (61)	182 (48)	107 (58)	94 (3)	255 (29)	230 (57)
G9	95 (56)	209 (24)	188 (5)	99 (5)	237 (39)	234 (35)
A10	104 (26)	244 (25)	180 (4)	95 (1)	207 (9)	312 (8)
A11	230 (73)	185 (30)	107 (50)	95 (3)	201 (6)	285 (6)
C12	298 (5)	183 (9)	60 (3)	87 (1)	215 (6)	286 (4)
U13	281 (5)	175 (6)	57 (2)	85 (1)	206 (3)	298 (2)
C14	292 (3)	169 (4)	60 (2)	85 (1)	203 (5)	281 (3)
C15	285 (6)	184 (8)	54 (2)	89 (1)	216 (6)	295 (4)
A-RNA[b]	292	178	54	82	207	289

[a] Mean values in degrees calculated with Curves+ for the 10 structures. The standard deviation are given between parentheses.

[b] Reference values for canonical RNA structure are *Nucleic Acids in Chemistry and Biology* (Eds.:G. M. Blackburn. M.J. Gait. D. Loakes. D. M. Williams). Oxford University Press. **1996**. Chapter 2.