Supporting Information for:

Comparison of Global Structure and Dynamics of Native and Unmodified $tRNA^{val}$

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5 pages with 4 tables and figures.

Table S1 Detailed Parameters for NMR experiments on tRNAs

2D ^{1}H-^{1}H NOESY parameters and experimental conditions

Sample	np	ni	nt	sw	sw1	T	Instrument	t_{mix}
Native *E. coli* tRNA^{val}								
2.2 mM tRNA, 10 mM Sodium Phosphate pH7.0, 80 mM NaCl, 5 mM $MgCl_2$, 0.1 mM EDTA, 10% D_2O	2048	400	64	13522	13500	25°C	600 MHz	200
Unmodified *E. coli* tRNA^{val}								
0.7 mM tRNA, 10 mM Sodium Phosphate pH7.0, 80 mM NaCl, 5 mM $MgCl_2$, 0.1 mM EDTA, 10% D_2O	4096	400	64	13522	13500	25°C	600 MHz	200

^{1}H-^{15}N HSQC parameters and experimental conditions

Sample	np	ni	nt	sw	sw1	T	Instrument
Native *E. coli* tRNA^{val}							
2.2 mM tRNA, 10 mM Sodium Phosphate pH7.0, 80 mM NaCl, 5 mM $MgCl_2$, 0.1 mM EDTA, 10% D_2O	2048	160	100	12001	3000	25°C	500 MHz
Unmodified *E. coli* tRNA^{val}							
0.7 mM tRNA, 10 mM Sodium Phosphate pH7.0, 80 mM NaCl, 5 mM $MgCl_2$, 0.1 mM EDTA, 10% D_2O	1024	200	48	14006	3000	25°C	600 MHz

^{1}H-^{15}N DSSE-HSQC parameters and experimental conditions

Sample	np	ni	nt	sw	sw1	T	Instrument	D_2O split
Native *E. coli* tRNA^{val}								
2.2 mM tRNA, 10 mM Sodium Phosphate pH7.0, 80 mM NaCl, 5 mM $MgCl_2$, 0.1 mM EDTA, 10% D_2O	4096	256	64	14006	3650	25°C	600 MHz	-
1.0 mM tRNA, 10 mM Sodium Phosphate pH7.0, 80 mM NaCl, 5 mM $MgCl_2$, 0.1 mM EDTA, 10% D_2O *+ C8E5/1-octanol*	4096	256	8	14006	3650	15°C	600 MHz	9.3
Unmodified *E. coli* tRNA^{val}								
0.7 mM tRNA, 10 mM Sodium Phosphate pH7.0, 80 mM NaCl, 5 mM $MgCl_2$, 0.1 mM EDTA, 10% D_2O	4096	256	64	14006	3650	25°C	600 MHz	-
0.3 mM tRNA, 10 mM Sodium Phosphate pH7.0, 80 mM NaCl, 5 mM $MgCl_2$, 0.1 mM EDTA, 10% D_2O *+ 15mg/ml Pf1*	4096	256	96	14006	3650	25°C	600 MHz	8.1

np - the number of complex points in the t_2 domain
ni - the number of complex points in the t_1 domain
nt - number of scans
sw - sweep width in Hz in t_2
sw1 - sweep width in Hz in t_1
t_{mix} - mixing time in milliseconds
T - temperature
D_2O split - the split of the deuterium of D_2O signal due to anisotropic averaging of the deuterium quadrupole moment

Table S2 Effect of varying magnitudes alignment tensor on the results of the domain orientation calculations for from *E. coli* native $tRNA^{val}$[a]

Alignment Tensor Parameters		Arm Orientation		
D_a (Hz)	**R**	**Bend (º)**	**Twist (º)**	**RDC rmsd**
15.0	0.55	101	178	5.89
16.0	0.55	102	179	5.64
17.0	0.55	103	179	5.56
18.0	0.55	105	179	5.62
19.0	0.55	106	179	5.85
17.0	0.40	99	181	5.81
17.0	0.45	100	181	5.67
17.0	0.50	102	180	5.58
17.0	0.60	105	178	5.59
17.0	0.65	107	177	5.69

[a] The magnitudes of the alignment tensor used as input for the domain orientation calculations.

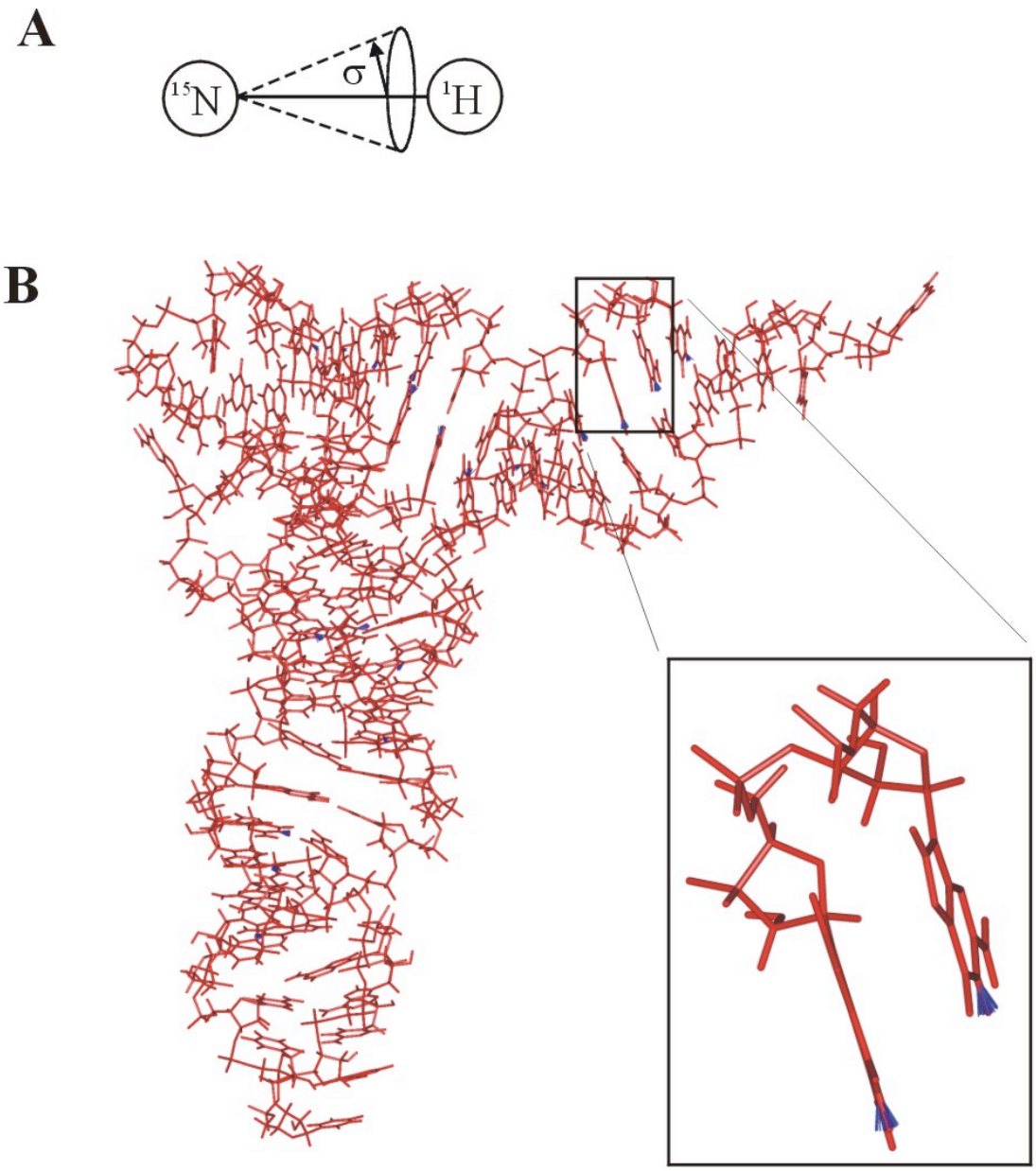

Figure S1 A) Diagram of an imino bond. Structural error was generated by moving only the proton of the imino bond within a cone where the angle of the cone is σ of a Gaussian distribution. B) Fifty structures with 10° structural error (σ=10°) in blue are superimposed on the A-form model tRNA (red). Inset shows close up of residues 2 and 3 to demonstrate that only the imino protons in the structure are moved to simulate structural error.

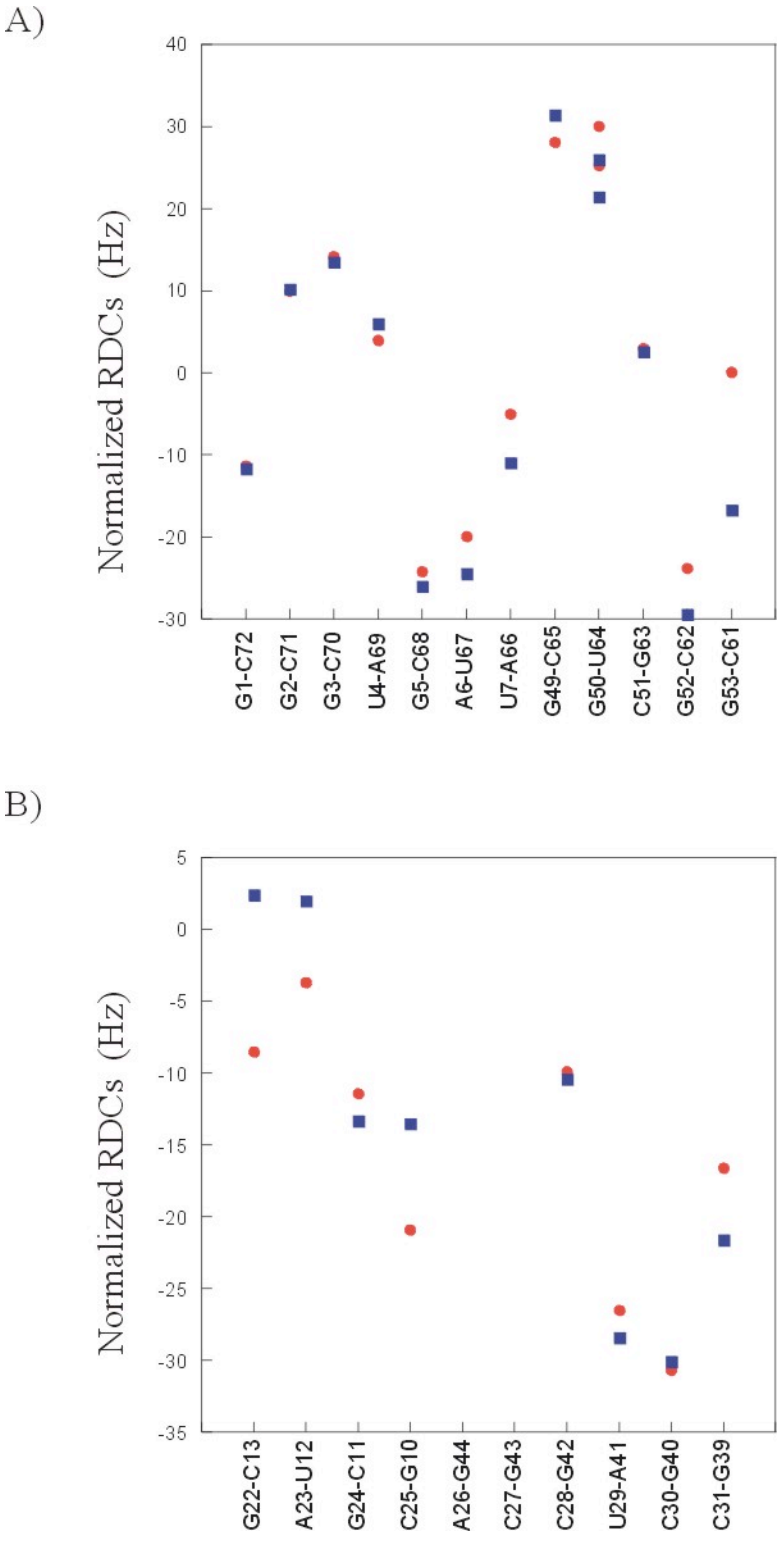

Figure S2. Normalized RDCs measured for native *E. coli* $tRNA^{val}$ in 5 mM Mg^{2+} at 15°C (blue squares) and unmodified *E. coli* $tRNA^{val}$ at 25°C (red circles) plotted as a function of position in (A) the acceptor arm and (B) the anticodon arm.