Table 6. Comparison of the thermodynamic parameters obtained for residues of Groups 1, 2, and 3 as defined in Tables 1 and 2

Group	Forward		Reverse		Equilibrium		Barrier ΔG^{+} at 22°C, kJ/mol	
	ΔH^{+}, kJ/mol	ΔS^{+}, J/mol K	ΔH^{+} kJ/mol	ΔS^{+}, J/mol K	ΔH, kJ/mol	ΔS, J/mol K	Forward	Reverse
1	72 ± 4	16 ± 14	62 ± 5	26 ± 17	9 ± 3	–9 ± 4	66.7 ± 0.1	54.8 ± 0.1
2	67 ± 1	15 ± 4	67 ± 3	32 ± 9	–1 ± 3	–16 ± 10	62.3 ± 0.1	58.0 ± 0.1
3	42 ± 2	–62 ± 6	62 ± 1	23 ± 4	–21 ± 1	–85 ± 4	60.1 ± 0.1	55.4 ± 0.1

Relaxation dispersion data were fit directly to a model where k_a and k_b were constrained according to the relation $k_{a/b} = \frac{k_B T}{h} \exp\left(-\Delta G^{+}_{a/b} / RT\right)$. Chemical shift differences were assumed to be temperature-independent. Note that in Tables 1 and 2, parameters were obtained from fits where rates were not constrained to a specific functional form and where temperature-independent $\Delta\varpi$ values were assumed.