Table 4. Comparison of the thermodynamic parameters obtained for residues of Groups 1, 2, and 3 as defined in Tables 1 and 2

	Forward		**Reverse**		**Equilibrium**		**Barrier ΔG^{+} at 22°C, kJ/mol**	
Group	**ΔH^{+}, kJ/mol**	**ΔS^{+}, J/mol K**	**ΔH^{+}, kJ/mol**	**ΔS^{+}, J/mol K**	**ΔH, kJ/mol**	**ΔS, J/mol K**	**Forward**	**Reverse**
1	75 ± 5	27 ± 15	70 ± 7	50 ± 22	5 ± 5	–23 ± 16	66.7 ± 0.1	54.8 ± 0.1
2	67 ± 2	17 ± 8	60 ± 4	8 ± 12	7 ± 4	9 ± 12	62.3 ± 0.1	57.9 ± 0.1
3	45 ± 4	–49 ± 13	60 ± 1	17 ± 5	–15 ± 4	–66 ± 13	59.8 ± 0.1	55.5 ± 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 between states *a* and *b*, $\Delta\varpi$, were allowed to vary with temperature. 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.