EMPIRICAL PREDICTIONS OF PROTEIN CONFORMATION

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Table 1 Conformational parameters for α-helical, β-sheet, and β-turn residues in 29 proteins[a]

P_α			P_β			P_t	f_i		f_{i+1}		f_{i+2}		f_{i+3}	
Glu	1.51	H_α	Val	1.70	H_β	Asn 1.56	Asn	0.161	Pro	0.301	Asn	0.191	Trp	0.167
Met	1.45		Ile	1.60		Gly 1.56	Cys	0.149	Ser	0.139	Gly	0.190	Gly	0.152
Ala	1.42		Tyr	1.47		Pro 1.52	Asp	0.147	Lys	0.115	Asp	0.179	Cys	0.128
Leu	1.21		Phe	1.38	h_β	Asp 1.46	His	0.140	Asp	0.110	Ser	0.125	Tyr	0.125
Lys	1.16	h_α	Trp	1.37		Ser 1.43	Ser	0.120	Thr	0.108	Cys	0.117	Ser	0.106
Phe	1.13		Leu	1.30		Cys 1.19	Pro	0.102	Arg	0.106	Tyr	0.114	Gln	0.098
Gln	1.11		Cys	1.19		Tyr 1.14	Gly	0.102	Gln	0.098	Arg	0.099	Lys	0.095
Trp	1.08		Thr	1.19		Lys 1.01	Thr	0.086	Gly	0.085	His	0.093	Asn	0.091
Ile	1.08		Gln	1.10		Gln 0.98	Tyr	0.082	Asn	0.083	Glu	0.077	Arg	0.085
Val	1.06		Met	1.05		Thr 0.96	Trp	0.077	Met	0.082	Lys	0.072	Asp	0.081
Asp	1.01	I_α	Arg	0.93	i_β	Trp 0.96	Gln	0.074	Ala	0.076	Thr	0.065	Thr	0.079
His	1.00		Asn	0.89		Arg 0.95	Arg	0.070	Tyr	0.065	Phe	0.065	Leu	0.070
Arg	0.98	i_α	His	0.87		His 0.95	Met	0.068	Glu	0.060	Trp	0.064	Pro	0.068
Thr	0.83		Ala	0.83		Glu 0.74	Val	0.062	Cys	0.053	Gln	0.037	Phe	0.065
Ser	0.77		Ser	0.75	b_β	Ala 0.66	Leu	0.061	Val	0.048	Leu	0.036	Glu	0.064
Cys	0.70		Gly	0.75		Met 0.60	Ala	0.060	His	0.047	Ala	0.035	Ala	0.058
Tyr	0.69	b_α	Lys	0.74		Phe 0.60	Phe	0.059	Phe	0.041	Pro	0.034	Ile	0.056
Asn	0.67		Pro	0.55	B_β	Leu 0.59	Glu	0.056	Ile	0.034	Val	0.028	Met	0.055
Pro	0.57	B_α	Asp	0.54		Val 0.50	Lys	0.055	Leu	0.025	Met	0.014	His	0.054
Gly	0.57		Glu	0.37		Ile 0.47	Ile	0.043	Trp	0.013	Ile	0.013	Val	0.053

[a] P_α, P_β, P_t are conformational parameters of helical, β-sheet, and β-turns. f_i, f_{i+1}, f_{i+2}, and f_{i+3} are bend frequencies in the four positions of the β-turn. H_α, H_β, etc, are as defined previously (25, 72). Bend frequencies are based on 408 β-turns (25).

A Thermodynamic Scale for the Helix-Forming Tendencies of the Commonly Occurring Amino Acids

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Table 2. Helix formation parameters for each of the 20 naturally occurring amino acids and Aib. The ΔG° values at 5 M urea were calculated from the relation $\Delta G^\circ = -RT\ln K_a$ with the value of K_a determined from the concentration dependence of dimerization for each peptide (Fig. 3). The $\Delta\Delta G_\alpha$ values were calculated by subtracting ΔG° for each peptide from ΔG° for the Gly-peptide. In contrast to the neutral amino acids, the values of $\Delta\Delta G_\alpha$ for the charged amino acids (*) were somewhat dependent on ionic strength and varied up to 0.3 kcal/mol between 0 and 1 M NaCl. The values cited refer to the values obtained directly in 1.0 M NaCl or extrapolated to 1.0 M NaCl. The values for P_{mid} are from (*4*), for P_α are from (*30*), and for s are from (*38*).

Amino acid	$\Delta\Delta G_\alpha$ (kcal/mol)	P_{mid}	P_α	s
Ala	−0.77	1.8	1.60	1.07
Aib	−0.69			
Arg	−0.68*	1.3	1.25	1.03
Lys	−0.65*	1.1	1.05	0.94
Leu	−0.62	1.2	1.50	1.14
Met	−0.50	1.5	1.44	1.20
Trp	−0.45	1.5	1.34	1.11
Phe	−0.41	1.3	1.45	1.09
Ser	−0.35	0.6	0.44	0.76
Gln	−0.33	1.3	1.22	0.98
Glu	−0.27*	0.8	1.18	0.97
Cys	−0.23	0.7	0.66	0.99
Ile	−0.23	1.2	1.31	1.14
Tyr	−0.17	0.8	0.61	1.02
Asp	−0.15*	1.0	1.03	0.68
Val	−0.14	1.2	1.09	0.95
Thr	−0.11	1.0	0.87	0.82
Asn	−0.07	0.9	0.80	0.78
His	−0.06*	1.0	0.97	0.69
Gly	0.00	0.5	0.47	0.59
Pro	~3	0.3	0.19	0.19

A Thermodynamic Scale for the β-Sheet Forming Tendencies of the Amino Acids

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Table 2: Summary of the β-Sheet Propensity Data[a]

guest residue	T_m (°C)	$\Delta\Delta G$ (kcal/mol)	P_β	$\Delta\Delta G_{(Kim\&Berg)}$ (kcal/mol)
Tyr	69.22	−1.63	1.31	−0.50
Thr	68.67	−1.36	1.33	−0.48
Ile	67.78	−1.25	1.57	−0.56
Phe	67.68	−1.08	1.23	−0.55
Trp	65.73	−1.04	1.24	−0.48
Val	65.47	−0.94	1.64	−0.53
Ser	64.80	−0.87	0.94	−0.39
Met	64.26	−0.90	1.01	−0.46
Cys	63.99	−0.78	1.07	−0.47
Leu	62.47	−0.45	1.17	−0.48
Arg	62.41	−0.40	0.94	−0.44
Asn	61.88	−0.52	0.66	−0.38
His	60.96	−0.37	0.83	−0.46
Gln	60.90	−0.38	1.00	−0.40
Lys	60.65	−0.35	0.73	−0.41
Glu	58.81	−0.23	0.51	−0.41
Ala	57.05	0	0.79	−0.35
Asp	50.91	0.85	0.66	−0.41
Gly	45.95	1.21	0.87	0
Pro	<10	ND	0.62	0.23

[a] The amino acids are listed in the order of their β-sheet propensity. The T_m of the thermal denaturation transition and $\Delta\Delta G$ relative to that of the standard, β1 T2Q, I6A, T44A, T53A, are included. $\Delta\Delta G$ for Pro was not determined (ND) for reasons discussed in the text. Absolute values are as follows: for T2Q, ΔG = −9.96 kcal/mol (T_m = 81.89 °C); for T2Q, I6A, ΔG = −7.05 kcal/mol (T_m = 71.12 °C); for T2Q, I6A, T44A, T53, ΔG = −6.54 kcal/mol (T_m = 68.73 °C); and for T2Q, I6A, T44A, T53A, ΔG = −4.62 kcal/mol (T_m = 57.05 °C). In the table, ΔG is determined by calculating ΔH in the transition region, using the van't Hoff equation and then using this value to calculate ΔS at the T_m. This treatment assumes that, within the transition region, ΔH is independent of temperature. Accordingly, $\Delta\Delta G$ values are reported at a temperature that is within the transition region for all the mutants (60 °C). For the standard β1 containing Ala at the guest site, ΔG = −0.24 kcal/mol at 60 °C. Also shown are the P_β values for the probability of occurence of each amino acid in β-sheet in proteins of known structure (Chou & Fasman, 1974, 1978) and the $\Delta\Delta G$ values from the Kim and Berg (1993) zinc finger study, which are relative to Gly at the guest postion.