

SUPPORTING INFORMATION

Modeling the Solvation of Nonpolar Amino Acids in Guanidinium Chloride Solutions

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Supplementary Table 1. Nonpolar amino acid residue ASA and solvation data.

amino acid	ASA (Å ²) ^a	GdmCl (M)			
		1	2	4	6
		ΔG_{solv} (cal/mol) ^b			
alanine	113	-40	-60	-50	-15
isoleucine ^c	182	-132	-223	-318	-406
leucine	180	-180	-245	-375	-450
methionine	204	-180	-285	-420	-505
phenylalanine	218	-240	-395	-600	-745
tryptophan	259	-425	-670	-1000	-1205
tyrosine	229	-265	-425	-625	-740
valine	160	-105	-258	-205	-212

^aBased on Gly-X-Gly from Miller et al.¹⁶

^bNozaki and Tanford⁹

^cSarker et al.¹²

Supplementary Table 2. NATA solvation data.^a

GdnHCl (M)	ΔG_{solv} (cal/mol)			
	15 °C	25 °C	35 °C	45 °C
0.4	-92	-131	-111	-139
0.8	-197	-232	-257	-290
1.2	-256	-301	-342	-421
1.6	-360	-390	-425	-491
2.0	-403	-471	-545	-605
2.4	-489	-559	-614	-692
2.8	-541	-622	-668	-763
3.2	-603	-707	-767	-868
3.4	-645	-709	-807	-885
3.8	-695	-780	-854	-945
4.2	-773	-802	-916	-1011
4.6	-793	-865	-995	-1076
5.0	-857	-887	-1022	-1086
5.4	-885	-989	-1066	-1136
6.0	-928	-1001	-1097	-1154

^aParker and Clarke¹¹