

Table 3. Optimized SPT implicit solvent nonpolar MF parameter values and goodness-of-fit metrics

Parameters	SPT component		
	SASA-only	SAV-only	Full SPT
σ_s , Å	2.2*	1.15 [1.01-1.27]	1.11 [1.00-1.26]
γ , cal·mol ⁻¹ ·Å ⁻²	17.1 (7)*	--	3 (1)
p , cal·mol ⁻¹ ·Å ⁻³	--	31.0 (9)	34 (1)
R	0.39*	0.77	0.78
R	0.63*	0.88	0.88
χ^2 , 10 ⁻³	19.6*	7.32	7.20
kcal ² ·mol ⁻² ·Å ⁻²			

Fits to the total explicit solvation force were performed for SASA-only, SAV-only, and full SPT forms of the implicit repulsive solvation MFs. Where applicable, standard errors are presented in parentheses; 99% confidence intervals are presented in brackets.

* σ_s parameters that reached the end (2.2 Å) of the search interval.