Table 2. *Coordinates, surface areas, and free energies*[a]

PDB file	Surface area (Å^2)	ΔG^0_{apolar} (kcal/mole)	ΔG^0_{polar} (kcal/mole)	ΔG^0_{assoc} (kcal/mole)	ΔG^0_{obs} (kcal/mole)	Ref.[b]
2PTC	1,465	−11.54	−8.65	−19.9	−18.1	a
1TPA	1,474	−10.82	−7.09	−17.1	−17.8	b
2KAI	1,471	−9.74	−4.74	−12.8	−12.4	c
4CPA	1,420	−10.13	−1.80	−10.0	−10.0	d
3CPA	594	−4.18	−5.04	−5.4	−5.3	e
3SGB	1,322	−11.02	−2.72	−12.3	−14.7	f
2SEC	1,547	−11.97	−2.72	−13.6	−13.1	g
1CSE	1,541	−12.14	−3.75	−15.0	−13.1	g
1CHO	1,547	−12.22	−3.55	−14.9	−15.7	h
2TPI	601	−5.56	−3.91	−6.1	−5.8	i
2TPI	1,457	−10.78	−7.36	−17.3	−18.1	i
1INS	1,305	−10.33	−1.24	−9.6	−7.4	j
2SSI	1,594	−12.78	−3.28	−15.4	−16	k
2HFL	1,775	−9.63	−4.64	−12.6	−14.2	l
1HBS	760	−7.84	−0.01	−4.7	−4.8	m

[a] Simple associations. The complexes are identified by the Brookhaven PDB code: 2PTC, trypsin–bovine pancreatic trypsin inhibitor (BPTI); 1TPA, anhydrotrypsin–BPTI; 2KAI, kallikrein A–BPTI; 4CPA, carboxypeptidase A–potato carboxypeptidase A inhibitor (PCI); 3CPA, carboxypeptidase A–glycyltyrosine; 3SGB, proteinase B–third domain of the turkey ovomucoid inhibitor (OMTK3); 2SEC, subtilisin Carlsberg–*N*-acetyl Eglin C; 1CSE, subtilisin Carlsberg–Eglin C; 1CHO, a-chymotrypsin–OMTKY3; 2TPI, trypsinogen (+BPTI)–isoleucylvaline (IV); 2TPI, trypsinogen (+IV)–BPTI; 1INS, insulin OP contact; 2SSI, *Streptomyces* subtilisin inhibitor dimer; 2HFL, lysozyme-Fab; 1HBS, sickle cell deoxyhemoglobin mol 1–2 contact.

[b] The experimental association energies were obtained from the literature. a, Vincent and Lazdunski (1972); b, Vincent et al. (1974); c, Chen and Bode (1983); d, Hass and Ryan (1980); e, Bunting and Myers (1975); f, Read et al. (1983); g, Ascenzi et al. (1988); h, Empie and Laskowski (1982); i, Bode (1979) and Bolognes et al. (1982); j, Pekar and Frank (1972); k, Akasaka et al. (1982); l, Sheriff et al. (1987); m, Ross et al. (1977).