Table 7. Sequence identities of minimum energy sequences selected by DESIGNER relative to their native counterparts, for several protein templates, in two types of design calculations

Fold	PDB ID	No. of sequences	All-best	All-min	Core-min	Surf-min
No composition imposed						
Ci2	2ci2	98	27.1	22.0	53.8	16.7
Cold-shock	1mjc	58	33.8	30.8	80.0	16.7
HTH	1r69	190	40.4	30.8	78.6	17.6
Native-like composition						
Ci2	2ci2	89	40.7	25.4	46.2	33.3
Cold-shock	1mjc	52	36.9	35.4	86.7	16.7
HTH	1r69	72	42.3	40.4	78.6	29.4

One type is without constraints imposed on the amino acid composition ("No composition imposed"), as described in the text, and the other where the amino acid composition was imposed to remain constant to that observed in the native sequence. Note that different calculations were performed with various schemes of amino acid composition constraints (e.g., average composition of the entire family of all natural sequences of the same fold), with very similar results. The protein domain name is given in the first column, and the PDB ID code of the backbone used in the design calculations is given in the second column. The number of computed sequences in each case is listed in the third column. "All-best" refers to the highest identity score of the full sequence obtained from amongst all sequences within the allowed energy window, selected by DESIGNER; "All-min" refers to the identity score of the minimum energy sequence selected by DESIGNER; "Core-min" and "Surf-min" refer to the identity scores of the minimum energy sequences computed over core and surface residues, respectively, with those defined as in the text.