

Table 1. List of proteins and polypeptides^a

No.	Protein	Reference	PDB	L	$\ln(k_f)$	CO, %	Abs_CO
1	α -helix ^b	Thompson et al. 1997	— ^b	21	15.5	10.4	2.2
2	β -hairpin ^c	Munoz et al. 1997	1PGB	16	12	25.8	4.1
3	WW domain ^d	Jager et al. 2001	1PIN	34	9.5	19.0	6.5
4	E3/E1-binding domain of dihydrolipoyl acyltransferase ^e	Spector and Raleigh 1999	2PDD	41	9.8	11.0 \pm 0.4	4.5 \pm 0.2
5	ACBP	Kragelund et al. 1995	2ABD	86	6.6	14.3 \pm 0.3	12.3 \pm 0.3
6	Cytochrome b562 ^f	Wittung-Stafshede et al. 1999	256B	106	12.2	7.5	7.9
7	Colicin E9 immunity protein	Ferguson et al. 1999	1IMQ	86	7.3	12.1	10.4
8	λ -Repressor	Burton et al. 1996	1LMB	80	8.5	9.4	7.5
9	Fibronectin ninth FN3 module	Plaxco et al. 1997	1FNF	90	-0.9	18.1	16.3
10	Twitchin	Clarke et al. 1999	1WIT	93	0.4	20.3	18.9
11	Tenascin (short form)	Clarke et al. 1997	1TEN	90 (89)	1.1	17.4	15.4
12	SH3 domain (a-spectrin)	Viguera et al. 1996	1SHG	62 (57)	1.4	19.1	10.9
13	SH3 domain (src)	Grantcharova and Baker 1997	1SRL	64 (56)	4	19.6	11.0
14	SH3-domain (PI3 kinase) ^g	Guijarro et al. 1998	1PNJ	90 (86)	-1.1	16.1	13.9
15	SH3-domain (fyn)	Plaxco et al. 1998a	1SHF	67 (59)	4.5	18.3	10.8
16	Photosystem I accessory protein	P. Bowers and D. Baker, unpubl.	1PSF	69	3.2	17.0	11.7
17	CspB (<i>Bacillus subtilis</i>)	Schindler et al. 1995	1CSP	67	7.0	16.4	11.0
		Perl et al. 1998			6.5		
18	CspB (<i>B. caldolyticus</i>)	Perl et al. 1998	1C9O	66	7.2	7.5	7.9
19	CspB (<i>Thermatoga maritima</i>)	Perl et al. 1998	1G6P	66	6.3	17.5 \pm 0.4	11.4 \pm 0.3
20	CspA	Reid et al. 1998	1MJC	69	5.3	16.0	11.0
21	Cyclophilin A	Ikura et al. 2000	1LOP	164	6.6	15.7	25.7
22	DNA-binding protein ^h	Guerois and Serrano 2000	1C8C	63	7	12.7	8.0
23	IgG binding domain of streptococcal protein L ⁱ	Kim et al. 2000	1HZ6	62	4.1	16.1	10.0
24	Protein G	McCallister et al. 2000	1PGB	57 (56)	6	17.3	9.7
25	FKBP12	Main et al. 1999	1FKB	107	1.5	17.7	18.9
26	Ci2	Jackson and Fersht 1991	2CI2	64	3.9	15.7	10.0
27	Activation domain procarboxypeptidase A2	Villegas et al. 1995	1AYE	80	6.8	16.7	13.4
28	Spliceosomal protein U1A ^j	Silow and Oliveberg 1997	1URN	102 (96)	5.8	16.9	16.2
29	Muscle-AcP ^k	Van Nuland et al. 1998a	1APS	98	-1.5	21.7 \pm 0.6	21.2 \pm 0.6

The columns in this table are as follows: Protein, name of protein; Ref, reference to the original article on folding and unfolding kinetics; PDB, Protein Data Bank entry (Bernstein et al. 1977); L, number of residues in the protein used in the experimental study, and (in parentheses) the number of residues that have defined three-dimensional coordinates and contribute to the relative contact order () calculations; $\ln(k_f)$, natural logarithm of the experimental folding rates in the water; and Abs_CO, absolute contact order.

^a The list of single-domain proteins and peptides that lack both disulfide bonds and covalent bonds to ligands is taken from Galzitskaya et al. 2003). If folding of some protein was investigated at different temperatures, the experiment at the temperature closest to 25°C is presented in the Table; we took the slowest phase that is not considered as *cis/trans* proline isomerization phase in the original paper. If the three-dimensional structure of a protein whose folding was studied experimentally was absent in PDB, but PDB contains the structure of its mutant or very close homolog, the latter was used in our CO calculations; this is mentioned in a corresponding footnote. If several PDB entries are available for some protein, the best refined full-length X-ray structure is used in our CO calculation; in the absence of X-ray structure, the averaged NMR structure is used; in the absence of such, CO was averaged over all NMR models (in this case, the standard deviation is given). Nos. 1–3 indicate short peptides; 4–33, proteins with two-state folding within the whole range of experimental conditions; and 34–57, proteins with multistate folding in water.

^b There is no PDB entry for the Ala-rich 21-residue α -helix studied; the ideal (Ala)₂₁ α -helix was used in our contact order calculation.

^c $\ln(k_f)$ value in water refers also to the midtransition point at 24°C

^d Small WW domain consisting of one β -sheet is considered as a peptide. $\ln(k_f)$ value refers to the temperature 41.7°C.

^e $\ln(k_f)$ value is the investigators' extrapolation of folding rate to 25°C.

^f Two-state folding is assumed by long extrapolation made by investigators.

^g Although the investigators of the experimental paper reported that the SH3 domain from PI3 kinase is 84 amino acids long, it was actually refolded by them with the additional two N-terminal residues and four C-terminal residues. The latter four are absent in the PDB entry.

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No.	Protein	Reference	PDB	<i>L</i>	$\ln(k_f)$	<i>CO</i> , %	<i>Abs_CO</i>
30	S6	Otzen and Oliveberg 1999	1RIS	101 (97)	5.9	18.9	18.4
31	<i>His</i> -containing phosphocarrier protein	Van Nuland et al. 1998b	1POH	85	2.7	17.6	15.0
32	N-terminal domain from L9	Kuhlman et al. 1998	1DIV	56	6.1	12.7	7.1
33	Villin 14T	Choe et al. 1998	2VIK	126	6.8	12.3	15.4
34	Apomyoglobin ^l	Cavagnero et al. 1999	1A6N	151	1.1	8.4	12.7
35	Colicin E7 immunity protein	Ferguson et al. 1999	1CEI	87 (85)	5.8	10.8	9.2
36	Cro protein	Laurents et al. 2000	2CRO	71 (65)	3.7	11.2	7.3
37	P16 protein	Tang et al. 1999	2ASE	156	3.5	5.3	8.3
38	Twitching Ig repeat 27	Fowler and Clarke 2001	1TIT	89	3.6	17.8	15.8
39	CD2, 1st domain	Parker et al. 1997	1HNG	98 (95)	1.8	16.9	16.0
40	Fibronectin tenth FN3 module	Cota and Clarke 2000	1FNF	94	5.5	16.5	15.5
41	IFABP from rat	Burns et al. 1998	1IFC	131	3.4	13.5	17.7
42	ILBP ^m	Dalessio and Ropson 2000	1EAL	127	1.3	12.3 ± 0.5	15.7 ± 0.6
43	CRBP II	Burns et al. 1998	1OPA	133	1.4	14.0	18.7
44	CRABP I	Burns et al. 1998	1CBI	136	-3.2	13.8	18.8
45	tryptophan synthase α -subunit ⁿ	Ogasahara and Yutani 1994	1QOP	268 (267)	-2.5	8.3	22.3
46	GroEL apical domain (191–345)	Golbik et al. 1998	1AON	155	0.8	13.7	21.2
47	Barstar ^o	Schreiber and Fersht 1993	1BRS	89	3.4	11.8	10.5
48	Che Y	Munoz et al. 1994	3CHY	129 (128)	1	8.7	11.2
49	Ribonuclease HI ^p	Parker and Marqusee 1999	2RN2	155	0.1	12.4	19.3
50	DHFR (dihydrofolate reductase) ^q	Jennings et al. 1993	1RA9	159	4.6	14.0	22.3
51	tryptophan synthase β_2 -subunit ⁿ	Goldberg et al. 1990	1QOP	396 (390)	-6.9	8.3	32.5
52	N-terminal domain from PGK	Parker et al. 1995	1PHP	175	2.3	11.5	20.2
53	C-terminal domain from PGK ^r	Parker et al. 1996	1PHP	219	-3.5	8.0	17.4
54	Barnase	Matouschek et al. 1990	1BNI	110 (108)	2.6	11.4	12.3
55	T4 lysozyme ^s	Parker and Marqusee 1999	2LZM	164	4.1	7.1	11.6
56	Ubiquitin ^t	Khorasanizadeh et al. 1996	1UBQ	76	5.9	15.1	11.5
57	Suc 1 ^u	Schymkowitz et al. 2000	1SCE	113 (101)	4.2	11.8	11.9

^h The folding of mutant protein Y34W was studied experimentally; we used the available PDB structure of wild type in our calculation of *CO*.

ⁱ The folding of mutant protein Y47W was studied experimentally; we used the available PDB structure of this mutant in our calculation of *CO*.

^j The folding of mutant protein F56W was studied experimentally; we used the available PDB structure of mutant Y31H/Q36R in our calculation of *CO*.

^k The folding of mutant protein C21S was studied experimentally; we used the available PDB structure of wild type protein in our calculation of *CO*.

^l We used the available PDB structure of a holoform of myoglobin (but without heme) in our calculation of *CO*.

^m We used the available PDB structure of mutant protein T118S from pig in our calculation of *CO* instead of the wild type protein from rat

ⁿ The folding of protein from *Escherichia coli* was studied experimentally. We used the available PDB structure of the same protein from *Salmonella typhimurium* in our calculation of *CO*.

^o The folding of mutant protein C40A/C82A was studied experimentally; we used the available PDB structure of this mutant in our calculation of *CO*.

^p The folding of mutant protein C13A/C63A/C133A was studied experimentally; we used the available PDB structure of wild type protein in our calculation of *CO*.

^q The folding of wild type protein was studied. We used the available PDB structure of mutant protein N37D in our calculation of *CO*. $\ln(k_f)$ value refers to the summary rate of two parallel pathways of refolding of DHFR.

^r The folding of mutant protein W290Y was studied experimentally. We used the available PDB structure of wild type in our calculation of *CO*.

^s The folding of Cys-free mutant was studied experimentally. We used the available PDB structure of wild-type protein in our calculation of *CO*.

^t The folding of bovine protein F45W mutant was studied experimentally. We used the available PDB structure of WT human protein in our calculation of *CO*.

^u There is only a strand-exchanged form of suc1 dimer in PDB. We used a concatenation of fragment 2–88 of chain C and fragment 89–102 of chain A as a tentative structure of monomeric protein in our calculation of *CO*.