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(Supporting Material)

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SHORT TITLE: Determination of Average RMSD from B-factors

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TABLE S1. Number of structures in clusters. Structures were clustered based on their pairwise RMSD values as described in the Methods. Clustering was done for two data sets - native and unfolded villin structures, and for two types of the alignment: pairwise alignment (PA) and alignment to a reference structure (RSA).

Cluster index	PA - native	RSA - native	PA - unfolded	RSA - unfolded
1	88	94	3	4
2	295	327	14	30
3	462	493	106	312
4	627	690	519	1129
5	672	764	1221	1939
6	678	774	1829	2220
7	710	803	2034	2193
8	696	749	1876	1864
9	748	777	1668	1699
10	958	1034	1454	1476
11	701	766	1141	1554
12	765	733	941	1255
13	785	900	918	922
14	737	775	902	577
15	729	742	890	241
16	701	740	659	142
17	620	739	335	68
18	638	408	72	28
19	265	99	23	14
20	25	12	4	6

Selection of X-ray Structures and RMSD Calculations

Structures used for calculations were downloaded from the RCSB Protein Data Bank on 11th May 2009 using the following search criteria: structures had to be solved by X-ray crystallography with resolution lower than 2.8 Å and refinement R_{free} factor lower than 0.2; they had to contain proteins, but no nucleic acids. We downloaded 4814 structures and from that data set we excluded structures that had non-physical, negative B-factors (3 structures). R_{struct} was calculated for every structure using Eq. 25 and $<RMSD^2>^{1/2}$ using Eq. 20 assuming $N_s>>1$. Calculations were done for backbone atoms and for all atoms. Both distributions of the calculated values were plotted.