Supporting information for Halle (January 29, 2002) *Proc. Natl. Acad. Sci. USA*, 10.1073/pnas.032522499.

Table 3. Quality indicators for model predictions of AMSD profiles for set of 38 nonhomologous proteins

	Density based on Cα atoms				Density based on nonhydrogen atoms (LDM)					
	Δ		ρ		Δ			ρ		
PDB	LDM*	GNM	LDM*	GNM	ref/fix†	ref/scd†	xtl/scd†	ref/fix†	ref/scd†	xtl/scd†
1RB9	1.31	1.57	0.42	0.34	1.25	1.21	0.88	0.41	0.43	0.52
2FDN	1.24	1.32	0.57	0.53	1.08	1.05	0.74	0.53	0.54	0.71
2KNT	0.80	0.74	0.62	0.78	0.68	0.64	0.67	0.75	0.76	0.71
2IGD	1.07	1.22	0.48	0.60	0.98	0.98	0.53	0.53	0.55	0.83
1G2B	1.06	1.20	0.67	0.66	1.08	1.07	0.70	0.69	0.69	0.74
1F94	2.32	3.06	0.60	0.53	2.19	2.09	1.13	0.63	0.65	0.71
1HG7	1.02	1.11	0.62	0.70	0.81	0.80	0.70	0.60	0.63	0.69
1C9O	1.38	1.74	0.52	0.54	1.39	1.36	0.77	0.55	0.58	0.71
1C75	1.18	1.64	0.52	0.24	1.02	0.94	0.71	0.64	0.67	0.73
1CC8	1.13	1.11	0.55	0.55	0.98	0.92	0.55	0.63	0.64	0.84
1B0Y	0.82	0.86	0.70	0.70	0.72	0.71	0.70	0.75	0.76	0.75
1CTJ	1.04	1.25	0.42	0.27	0.92	0.88	0.75	0.51	0.54	0.56
1C5E	0.80	0.98	0.61	0.62	0.87	0.82	0.74	0.59	0.62	0.72
1RGE	1.04	1.33	0.66	0.54	0.93	0.94	0.70	0.66	0.67	0.74
1PSR	0.71	0.78	0.54	0.53	0.72	0.71	0.73	0.59	0.61	0.57
1JHG	0.99	1.28	0.52	0.05	0.86	0.85	0.70	0.54	0.55	0.71
2PVB	1.13	1.36	0.52	0.42	1.08	1.05	0.91	0.58	0.58	0.57

1DY5	1.05	1.05	0.54	0.63	1.01	0.97	0.71	0.55	0.56	0.64
3LZT	0.79	0.76	0.63	0.72	0.76	0.74	0.78	0.66	0.68	0.59
1CXQ	0.70	0.80	0.55	0.40	0.66	0.65	0.58	0.60	0.62	0.74
1QDD	0.69	0.77	0.69	0.76	0.65	0.63	0.67	0.76	0.78	0.83
1A6M	0.83	0.78	0.60	0.67	0.85	0.82	0.86	0.54	0.57	0.49
1MFM	0.91	0.96	0.48	0.46	0.82	0.80	0.72	0.58	0.59	0.72
1EQO	0.94	0.97	0.52	0.61	0.84	0.82	0.83	0.55	0.59	0.59
1CEX	0.73	0.69	0.73	0.80	0.67	0.66	0.65	0.80	0.81	0.85
1G66	0.76	0.84	0.63	0.66	0.70	0.69	0.63	0.69	0.70	0.76
1MUN	0.87	1.06	0.52	0.34	0.81	0.77	0.70	0.56	0.60	0.70
1FCY	0.85	0.88	0.66	0.68	0.77	0.72	0.65	0.68	0.72	0.74
1QL0	0.75	0.78	0.69	0.73	0.63	0.62	0.54	0.74	0.76	0.82
1QJ4	1.03	1.16	0.58	0.63	0.96	0.92	0.80	0.61	0.63	0.67
1GCI	0.99	0.96	0.69	0.77	0.75	0.72	0.63	0.73	0.75	0.76
1DCS	0.89	0.97	0.49	0.52	0.86	0.84	0.68	0.49	0.51	0.67
1QTW	0.81	0.84	0.58	0.62	0.78	0.75	0.77	0.64	0.68	0.68
1IXH	0.85	0.82	0.59	0.70	0.81	0.79	0.76	0.66	0.68	0.70
1BXO	0.84	0.87	0.70	0.79	0.79	0.76	0.71	0.76	0.78	0.78
1BG6	0.83	0.91	0.52	0.51	0.79	0.77	0.79	0.55	0.59	0.61
1C0P	0.86	0.80	0.50	0.63	0.77	0.76	0.78	0.62	0.65	0.65
3SIL	0.68	0.65	0.75	0.84	0.64	0.62	0.67	0.76	0.78	0.77

In all calculations, the cutoff radius R_C was set equal to the distance, $R_{\alpha\alpha}^{(2)}$, of the second minimum in the Cα - Cα radial density. PDB, Protein Data Bank identification code; LDM, local density model; GNM, Gaussian network model.

* Contact density is based on Cα atoms in reference molecule and calculated with self-consistently distributed atoms.

† Contact density is based on nonhydrogen atoms in reference molecule (ref) or entire crystal (xtl) and is calculated with fixed (fix) or self-consistently distributed (scd) atoms.