

Supplementary Table Comparison of diffraction-component precision index as generated by Cruickshank's formulae, and by equations (7) to (10).

protein	PDB accession	N_i *	s +	V_a A^3	V_M A^3/dalton +	d_{\min} A *	n_{obs} *	C *	R *	R_{free} *	DPI based on R_{free}			DPI based on R		
											Cruickshank	eq. (7)	eq. (9)	Cruickshank	eq. (8)	eq.(10)
											A	A	A	A	A	A
crambin	1CBN	447	0.28	8414	1.777	0.83	23759	0.81	0.090				0.012	0.0116	0.0109	
rubredoxin	8RXN	479	0.23	9592	1.680	1.00	18532	0.90	0.160				0.028	0.028	0.029	
ribonuclease MGMP	1RGE	1958	0.29	52781	2.418	1.15	62845	0.87	0.109				0.027	0.025	0.025	
ribonuclease MSA	1RGH	1832	0.23	49568	2.343	1.20	60670	0.95	0.106				0.026	0.023	0.025	
plastocyanin 295	1PLC	849	0.15	19974	1.905	1.33	14303	0.76	0.149				0.061	0.059	0.063	
plastocyanin 173S	1PNC	928	0.25	19127	1.824	1.60	7393	0.69	0.132				0.120	0.116	0.132	
plastocyanin 173H	#	911	0.23	19127	1.824	1.60	7393	0.69	0.153				0.136	0.132	0.150	
TGF-beta2 1TGI	2TGI	948	0.07	39913	3.138	1.80	14000	1.00	0.173				0.095	0.096	0.094	
TGF-beta2 1TFG	1TFG	974	0.09	39860	3.134	1.95	11000	1.00	0.188				0.136	0.137	0.135	
Cd-azurin	1AIZ	2215	0.12	69389	2.480	1.80	23366	0.94	0.168				0.121	0.121	0.120	
lactoferrin	1LFG	5907	0.09	212505	2.785	2.20	39506	0.90	0.179				0.252	0.245	0.264	
thaumatin C2	1THU	1552	0	50083	2.238	2.60	4622	0.75	0.184				@	@	@	
concanavalin A	1NLS	2130	0.18	60095	2.344	0.94	116712	0.75	0.128	0.148	0.021	0.020	0.021	0.020	0.0184	0.0188
HEWlysozyme gr	193L	1145	0.14	29123	2.053	1.33	24111	0.87	0.184	0.226	0.069	0.067	0.071	0.062	0.061	0.065
HEWlysozyme sp	194L	1141	0.14	29197	2.058	1.40	21542	0.89	0.183	0.226	0.076	0.074	0.079	0.069	0.067	0.073
gammaB crystallin	1GCS	1708	0.16	40523	1.982	1.49	26151	0.91	0.180	0.204	0.080	0.077	0.084	0.082	0.079	0.088
betaB2 crystallin	2BB2	1558	0.06	88700	4.280	2.10	18583	0.91	0.184	0.200	0.126	0.125	0.127	0.142	0.141	0.144
beta purothionin	1BHP	439	0.21	13229	2.685	1.70	4966	0.86	0.198	0.281	0.149	0.148	0.148	0.131	0.130	0.129
alpha1 purothionin	2PLH	434	0.31	12527	2.596	2.50	1168	0.61	0.155	0.218	0.392	0.375	0.426	@	@	@
EM lysozyme	1JUG	1068	0.06	29679	2.121	1.90	8308	0.89	0.169	0.229	0.162	0.161	0.164	0.172	0.170	0.175
azurin II	1ARN	1012	0.05	34869	2.531	1.90	12162	0.62	0.188	0.207	0.133	0.108	0.182	0.148	0.121	0.270
corrected\$							7210				0.173	0.168	0.182	0.237	0.230	0.270
rnase A + RI	1DFJ	4416	0.01	192570	3.072	2.50	18859	0.67	0.194	0.286	0.396	0.384	0.418	1.067	@	@
FabHyHEL-5 + HEW	2IFF	4333	0.02	158392	2.649	2.65	11754	0.73	0.196	0.288	0.515	0.532	0.489	@	@	@

* Values as given by Cruickshank (1999).

+ Using data deposited in PDB where not available from original publication. Molecular weight calculated from amino-acid sequence where necessary.

Not in protein data bank, see Fields et al. [(1994) Acta Cryst. D50, 709-730].

\$ Dodd et al. [(1995) Acta Cryst. D51, 1052-1064] quoted number of reflections "including anomalous", used by Cruickshank (1999).

Revised number of independent reflections calculated from Dodd et al., Table 1.

@ The number of free parameters p is negative.