Structure dataset	Binding ligand											
	ADP		***ATP***		***FAD***		***NAD***		***SAH***		***SAM***	
	PCC[a]	*MSE*[b]	*PCC*[a]	*MSE*[b]	*PCC*[a]	*MSE*[b]	*PCC*[a]	*MSE*[b]	*PCC*[a]	*MSE*[b]	*PCC*[a]	*MSE*[b]
Crystal structures	0.79	6.4	0.73	8.1	0.96	2.4	0.89	4.6	0.95	1.6	0.76	7.2
High-quality models	0.75	7.3	0.72	8.6	0.92	4.6	0.86	6.1	0.94	1.9	0.88	3.6
Moderate-quality models	0.75	7.9	0.68	10.1	0.88	7.2	0.86	6.3	0.86	4.1	0.83	4.9
Distorted to 2Å RMSD	0.75	7.6	0.68	9.6	0.93	4.3	0.88	5.2	0.94	2.0	0.86	4.4
Distorted to 4Å RMSD	0.69	8.7	0.68	9.7	0.88	6.7	0.84	6.9	0.86	4.4	0.83	4.9
Distorted to 6Å RMSD	0.60	10.9	0.68	10.0	0.83	8.5	0.81	7.3	0.85	4.4	0.76	7.5

[a] Pearson correlation coefficient. [b] Mean squared error in Å.