Dataset	Global similarity		Binding site matching			
	Sequence	***Structure***	***eMatchSite***	***PocketMatch***	***SiteEngine***	***sup-CK***
SOIPPA						
Crystal[a]	0.553	0.657	0.941	0.603	0.933	-
HQ models[b]	0.553	0.655	0.953	0.615	0.893	-
MQ models[c]	0.564	0.671	0.987	0.627	0.856	-
2Å RMSD[d]	0.553	0.653	0.948	0.616	0.911	-
4Å RMSD[d]	0.553	0.659	0.954	0.622	0.880	-
6Å RMSD[d]	0.556	0.660	0.948	0.610	0.889	-
Kahraman						
Crystal[a]	0.528	0.514	0.693	0.523	0.660	0.657
HQ models[b]	0.528	0.542	0.702	0.542	0.605	0.578
MQ models[c]	0.528	0.505	0.675	0.536	0.594	0.569
Homogeneous						
Crystal[a]	0.603	0.835	0.924	0.736	0.760	0.812
HQ models[b]	0.603	0.810	0.910	0.700	0.605	0.751
MQ models[c]	0.603	0.808	0.957	0.707	0.571	0.656
Steroid						
Crystal[a]	0.434	0.621	0.663	0.531	0.550	-
HQ models[b]	0.431	0.549	0.667	0.520	0.598	-
MQ models[c]	0.440	0.529	0.678	0.476	0.413	-

[a] Crystal structures. [b] High-quality protein models. [c] Moderate-quality protein models. [d] Structures artificially distorted to a desired Cα-RMSD.