

PDB ID	Fract. of surface covered by critical residues	Fract. of surface covered by known ligand-binding residues	Jaccard overlap btwn [critical reidues on surface] & [known lig-binding residues on surface]	# of distinct surface-critical sites	# of known ligand-binding sites	# of strongly overlapping sites (i.e., captured known lig-binding sites)	Fract. of known ligand-binding sites captured
3pfk	0.51	0.204	0.255 (0.155)	19	3	3	1
4ake	0.454	0.178	0.274 (0.154)	29	2	2	1
1cd5	0.589	0.1	0.153 (0.096)	24	2	1	0.5
1j3h	0.066	0.08	0.25 (0.041)	2	1	1	1
1bks	0.343	0.097	0.079 (0.079)	24	4	1	0.25
1e5x	0.207	0.093	0.139 (0.077)	17	3	2	0.667
1efk	0.055	0.086	0.03 (0.036)	10	10	0	0
1nr7	0.149	0.175	0.187 (0.102)	45	24	6	0.25
1xtt	0.298	0.196	0.295 (0.154)	31	5	5	1
2hnp	0.739	0.133	0.16 (0.134)	25	2	2	1
3d7s	0.267	0.137	0.054 (0.064)	26	9	0	0
3ju5	0.016	0.039	0 (0.013)	1	2	0	0
<i>mean</i>	0.308	0.127	0.156 (0.092)	21.083	5.583	1.917	0.556