Supplementary Table R3-Q11-1. Mann-Whitney test comparison between the predictions using native poses and the predictions using all the poses

We have compared the distribution of predicted values using the native poses against the distribution of predicted values using all the poses by doing a Mann-Whitney test. This was done for the predicted values of every predicted ratio, and for all the docking scores. In the table, we show the resulting p-value and estimate of the Mann-Whitney test.

	δ (KCal/mol)	AB2		AB2 Rigid		AB2 Flexible	
		p-value	estimate	p-value	estimate	p-value	estimate
FiberDock	δ ≤1.4	4.39E-01	0.1659	6.35E-01	0.1601	6.94E-01	0.1724
	1.4<δ≤2.8	8.47E-01	0.0871	5.09E-01	0.2186	4.13E-01	-0.5728
	2.8<δ≤4.2	8.22E-01	-0.1336	9.78E-01	-0.0315	8.00E-01	0.8794
	δ >4.2	6.16E-01	-0.1624	7.31E-01	0.1061	2.82E-01	-0.6036
aVdW	δ ≤1.4	6.09E-01	-0.0838	2.92E-01	0.2189	1.25E-01	-0.3454
	1.4<δ≤2.8	3.73E-01	0.2039	1.51E-01	0.6568	8.02E-01	-0.0565
	2.8<δ≤4.2	7.73E-01	0.0948	4.18E-01	0.2071	6.99E-01	-0.3848
	δ >4.2	1.06E-01	0.4227	6.66E-04	0.7996	4.85E-01	-0.2077
rVdW	δ ≤1.4	1.86E-01	0.0390	3.46E-04	0.1242	1.46E-01	-0.1532
	1.4<δ≤2.8	8.17E-01	0.0230	2.45E-01	0.0902	5.20E-01	-0.0999
	2.8<δ≤4.2	2.25E-02	0.1101	1.23E-01	0.0386	1.04E-01	0.2128
	δ >4.2	1.61E-04	0.2586	1.11E-04	0.3294	3.39E-01	0.0475
aElec	δ ≤1.4	4.57E-01	0.2068	2.14E-01	0.3377	8.99E-01	-0.0239
	1.4<δ≤2.8	8.29E-01	-0.1739	9.25E-01	0.0554	8.23E-01	-0.3118
	2.8<δ≤4.2	5.59E-01	-0.1150	9.75E-01	0.0062	1.81E-01	-0.3289
	δ >4.2	1.04E-02	0.2832	5.41E-04	0.5736	7.72E-01	0.0245
rElec	δ ≤1.4	2.05E-01	0.1963	2.64E-01	0.2343	4.03E-01	0.1730
	1.4<δ≤2.8	5.10E-01	0.0727	3.24E-01	0.4334	8.14E-01	-0.4879
	2.8<δ≤4.2	3.34E-01	-0.1741	8.17E-01	-0.0538	6.03E-02	-0.3167
	δ >4.2	1.36E-02	0.1742	5.79E-04	0.5405	8.60E-01	0.0091
laElec	δ ≤1.4	5.52E-01	0.1653	2.63E-01	0.2844	8.79E-01	-0.0289
	1.4<δ≤2.8	8.71E-01	-0.1023	8.41E-01	0.0097	6.73E-01	-0.1023
	2.8<δ≤4.2	3.39E-01	-0.1330	9.08E-01	-0.0481	5.97E-02	-0.4256
	δ >4.2	2.91E-02	0.2877	6.52E-04	0.5897	8.98E-01	-0.0196
lrElec	δ ≤1.4	7.75E-02	0.3277	1.59E-02	0.4292	8.16E-01	0.2153
	1.4<δ≤2.8	8.47E-01	-0.2850	1.00E+00	-0.0593	7.71E-01	-0.3682
	2.8<δ≤4.2	5.33E-01	-0.0958	6.39E-01	0.0565	1.38E-02	-0.2579
	δ >4.2	3.89E-03	0.3528	6.52E-04	0.7255	5.13E-01	0.1532
HB	δ ≤1.4	3.54E-01	0.1274	7.37E-01	-0.1160	1.26E-01	0.2520
	1.4<δ≤2.8	8.50E-02	0.2249	5.92E-01	0.1875	5.37E-02	0.2705
	2.8<δ≤4.2	1.06E-02	0.4828	2.32E-01	0.1992	2.89E-02	0.6348
	δ >4.2	4.78E-02	-0.2825	8.05E-02	-0.3906	7.55E-01	-0.0501
EPAIR	δ ≤1.4	7.51E-01	0.0867	4.93E-01	0.2796	9.44E-01	-0.0117
	1.4<δ≤2.8	3.00E-01	-0.2108	3.13E-01	-0.4230	7.23E-01	-0.0404
	2.8<δ≤4.2	1.66E-01	-0.3304	8.68E-01	0.0740	7.27E-02	-0.7724
	δ >4.2	5.02E-01	0.1877	6.31E-01	-0.1127	5.05E-03	0.5558
ES3DC	δ ≤1.4	6.41E-01	-0.1171	9.61E-01	0.0270	4.90E-01	-0.2321
	1.4<δ≤2.8	6.20E-01	-0.1792	6.10E-01	-0.2443	5.67E-01	-0.2393
	2.8<δ≤4.2	9.40E-01	0.1014	1.73E-01	1.0079	2.86E-01	-1.1376
	δ >4.2	6.08E-01	0.1281	3.21E-01	0.2410	8.36E-01	-0.3147
E3D	δ ≤1.4	7.84E-01	0.0445	5.72E-01	0.1402	8.35E-01	-0.0613
	1.4<δ≤2.8	8.35E-01	-0.0332	5.71E-01	0.5519	4.04E-01	-0.1367
	2.8<δ≤4.2	6.47E-02	0.2540	1.37E-02	0.2875	7.24E-01	-0.1469
	δ >4.2	7.67E-01	-0.0669	8.75E-01	0.0303	3.94E-01	-0.4570