**Supplementary Table R3-Q11-2. 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 predictions when δ is smaller or equal than 2.8 Kcal/mol, and when δ is greater than 2.8 Kcal/mol, and for all the docking scores. In the table, we show the resulting p-value and estimate of the Mann-Whitney test.

| | δ | AB2 | | AB2 Rigid | | AB2 Flexible | |
|---|---|---|---|---|---|---|---|
| | (KCal/mol) | p-value | estimate | p-value | estimate | p-value | estimate |
| FiberDock | δ ≤2.8 | 5.12E-01 | 0.1332 | 3.60E-01 | 0.2562 | 8.65E-01 | -0.0498 |
| | δ >2.8 | 5.17E-01 | -0.1542 | 7.72E-01 | 0.0883 | 2.11E-01 | -0.4965 |
| aVdW | δ ≤2.8 | 8.26E-01 | 0.0281 | 6.12E-02 | 0.3426 | 1.69E-01 | -0.2385 |
| | δ >2.8 | 2.23E-01 | 0.2080 | 6.35E-03 | 0.4513 | 2.19E-01 | -0.3907 |
| rVdW | δ ≤2.8 | 2.52E-01 | 0.0389 | 5.47E-04 | 0.1104 | 1.44E-01 | -0.1065 |
| | δ >2.8 | 1.31E-05 | 0.1520 | 8.74E-05 | 0.1548 | 5.43E-02 | 0.1101 |
| aElec | δ ≤2.8 | 6.76E-01 | 0.0442 | 3.44E-01 | 0.2801 | 7.56E-01 | -0.0322 |
| | δ >2.8 | 1.19E-01 | 0.1536 | 4.41E-02 | 0.4028 | 9.24E-01 | -0.1112 |
| rElec | δ ≤2.8 | 1.49E-01 | 0.1523 | 1.19E-01 | 0.3280 | 5.88E-01 | 0.0728 |
| | δ >2.8 | 3.02E-01 | 0.0696 | 1.30E-01 | 0.4417 | 7.28E-01 | -0.0318 |
| laElec | δ ≤2.8 | 6.74E-01 | 0.0411 | 2.16E-01 | 0.2829 | 6.16E-01 | -0.0513 |
| | δ >2.8 | 3.36E-01 | 0.1133 | 5.94E-02 | 0.4039 | 1.91E-01 | -0.1521 |
| lrElec | δ ≤2.8 | 2.45E-01 | 0.2179 | 1.04E-01 | 0.2776 | 1.00E+00 | 0.0709 |
| | δ >2.8 | 7.89E-02 | 0.1902 | 1.08E-02 | 0.5740 | 5.86E-01 | -0.0887 |
| HB | δ ≤2.8 | 5.38E-02 | 0.1964 | 7.83E-01 | 0.0963 | 1.30E-02 | 0.2629 |
| | δ >2.8 | 8.12E-01 | 0.0478 | 3.64E-01 | -0.1108 | 1.57E-01 | 0.3375 |
| EPAIR | δ ≤2.8 | 6.80E-01 | -0.0517 | 8.43E-01 | -0.0842 | 7.34E-01 | -0.0393 |
| | δ >2.8 | 6.52E-01 | -0.0763 | 7.53E-01 | -0.0446 | 9.76E-01 | -0.0148 |
| ES3DC | δ ≤2.8 | 5.32E-01 | -0.1241 | 8.80E-01 | -0.0434 | 4.07E-01 | -0.2059 |
| | δ >2.8 | 4.48E-01 | 0.1888 | 7.13E-02 | 0.6606 | 3.65E-01 | -0.5838 |
| E3D | δ ≤2.8 | 9.10E-01 | 0.0132 | 3.62E-01 | 0.2726 | 4.73E-01 | -0.0969 |
| | δ >2.8 | 2.25E-01 | 0.1445 | 2.49E-02 | 0.2090 | 2.91E-01 | -0.3836 |