**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 | 1.4 | 4.39E-01 | 0.1659 | 6.35E-01 | 0.1601 | 6.94E-01 | 0.1724 |
| 1.4δ2.8 | 8.47E-01 | 0.0871 | 5.09E-01 | 0.2186 | 4.13E-01 | -0.5728 |
| 2.8δ4.2 | 8.22E-01 | -0.1336 | 9.78E-01 | -0.0315 | 8.00E-01 | 0.8794 |
| 4.2 | 6.16E-01 | -0.1624 | 7.31E-01 | 0.1061 | 2.82E-01 | -0.6036 |
| aVdW | 1.4 | 6.09E-01 | -0.0838 | 2.92E-01 | 0.2189 | 1.25E-01 | -0.3454 |
| 1.4δ2.8 | 3.73E-01 | 0.2039 | 1.51E-01 | 0.6568 | 8.02E-01 | -0.0565 |
| 2.8δ4.2 | 7.73E-01 | 0.0948 | 4.18E-01 | 0.2071 | 6.99E-01 | -0.3848 |
| 4.2 | 1.06E-01 | 0.4227 | 6.66E-04 | 0.7996 | 4.85E-01 | -0.2077 |
| rVdW | 1.4 | 1.86E-01 | 0.0390 | 3.46E-04 | 0.1242 | 1.46E-01 | -0.1532 |
| 1.4δ2.8 | 8.17E-01 | 0.0230 | 2.45E-01 | 0.0902 | 5.20E-01 | -0.0999 |
| 2.8δ4.2 | 2.25E-02 | 0.1101 | 1.23E-01 | 0.0386 | 1.04E-01 | 0.2128 |
| 4.2 | 1.61E-04 | 0.2586 | 1.11E-04 | 0.3294 | 3.39E-01 | 0.0475 |
| aElec | 1.4 | 4.57E-01 | 0.2068 | 2.14E-01 | 0.3377 | 8.99E-01 | -0.0239 |
| 1.4δ2.8 | 8.29E-01 | -0.1739 | 9.25E-01 | 0.0554 | 8.23E-01 | -0.3118 |
| 2.8δ4.2 | 5.59E-01 | -0.1150 | 9.75E-01 | 0.0062 | 1.81E-01 | -0.3289 |
| 4.2 | 1.04E-02 | 0.2832 | 5.41E-04 | 0.5736 | 7.72E-01 | 0.0245 |
| rElec | 1.4 | 2.05E-01 | 0.1963 | 2.64E-01 | 0.2343 | 4.03E-01 | 0.1730 |
| 1.4δ2.8 | 5.10E-01 | 0.0727 | 3.24E-01 | 0.4334 | 8.14E-01 | -0.4879 |
| 2.8δ4.2 | 3.34E-01 | -0.1741 | 8.17E-01 | -0.0538 | 6.03E-02 | -0.3167 |
| 4.2 | 1.36E-02 | 0.1742 | 5.79E-04 | 0.5405 | 8.60E-01 | 0.0091 |
| laElec | 1.4 | 5.52E-01 | 0.1653 | 2.63E-01 | 0.2844 | 8.79E-01 | -0.0289 |
| 1.4δ2.8 | 8.71E-01 | -0.1023 | 8.41E-01 | 0.0097 | 6.73E-01 | -0.1023 |
| 2.8δ4.2 | 3.39E-01 | -0.1330 | 9.08E-01 | -0.0481 | 5.97E-02 | -0.4256 |
| 4.2 | 2.91E-02 | 0.2877 | 6.52E-04 | 0.5897 | 8.98E-01 | -0.0196 |
| lrElec | 1.4 | 7.75E-02 | 0.3277 | 1.59E-02 | 0.4292 | 8.16E-01 | 0.2153 |
| 1.4δ2.8 | 8.47E-01 | -0.2850 | 1.00E+00 | -0.0593 | 7.71E-01 | -0.3682 |
| 2.8δ4.2 | 5.33E-01 | -0.0958 | 6.39E-01 | 0.0565 | 1.38E-02 | -0.2579 |
| 4.2 | 3.89E-03 | 0.3528 | 6.52E-04 | 0.7255 | 5.13E-01 | 0.1532 |
| HB | 1.4 | 3.54E-01 | 0.1274 | 7.37E-01 | -0.1160 | 1.26E-01 | 0.2520 |
| 1.4δ2.8 | 8.50E-02 | 0.2249 | 5.92E-01 | 0.1875 | 5.37E-02 | 0.2705 |
| 2.8δ4.2 | 1.06E-02 | 0.4828 | 2.32E-01 | 0.1992 | 2.89E-02 | 0.6348 |
| 4.2 | 4.78E-02 | -0.2825 | 8.05E-02 | -0.3906 | 7.55E-01 | -0.0501 |
| EPAIR | 1.4 | 7.51E-01 | 0.0867 | 4.93E-01 | 0.2796 | 9.44E-01 | -0.0117 |
| 1.4δ2.8 | 3.00E-01 | -0.2108 | 3.13E-01 | -0.4230 | 7.23E-01 | -0.0404 |
| 2.8δ4.2 | 1.66E-01 | -0.3304 | 8.68E-01 | 0.0740 | 7.27E-02 | -0.7724 |
| 4.2 | 5.02E-01 | 0.1877 | 6.31E-01 | -0.1127 | 5.05E-03 | 0.5558 |
| ES3DC | 1.4 | 6.41E-01 | -0.1171 | 9.61E-01 | 0.0270 | 4.90E-01 | -0.2321 |
| 1.4δ2.8 | 6.20E-01 | -0.1792 | 6.10E-01 | -0.2443 | 5.67E-01 | -0.2393 |
| 2.8δ4.2 | 9.40E-01 | 0.1014 | 1.73E-01 | 1.0079 | 2.86E-01 | -1.1376 |
| 4.2 | 6.08E-01 | 0.1281 | 3.21E-01 | 0.2410 | 8.36E-01 | -0.3147 |
| E3D | 1.4 | 7.84E-01 | 0.0445 | 5.72E-01 | 0.1402 | 8.35E-01 | -0.0613 |
| 1.4δ2.8 | 8.35E-01 | -0.0332 | 5.71E-01 | 0.5519 | 4.04E-01 | -0.1367 |
| 2.8δ4.2 | 6.47E-02 | 0.2540 | 1.37E-02 | 0.2875 | 7.24E-01 | -0.1469 |
| 4.2 | 7.67E-01 | -0.0669 | 8.75E-01 | 0.0303 | 3.94E-01 | -0.4570 |