**Table S3.** **Binding site hit rates and bound state similarity coefficients (BSSCs) for the ensemble of ligand-free MAGI-1 PDZ1 structures (PDB ID 1kpk). The BSSC values are calculated using the ligand-bound structure with PDB IDs 2kpl. The models are sorted based on the hit rate. The maximum value in each column is shown in bold.**

|  |  |  |
| --- | --- | --- |
| **Model** | **HR** |  **BSSC** |
| 7 | **0.81** | 0.52 |
| 17 | 0.81 | 0.50 |
| 9 | 0.79 | **0.58** |
| 13 | 0.78 | 0.52 |
| 6 | 0.74 | 0.51 |
| 5 | 0.68 | 0.48 |
| 2 | 0.66 | 0.51 |
| 18 | 0.66 | 0.50 |
| 4 | 0.63 | 0.49 |
| 10 | 0.63 | 0.54 |
| Average | 0.63 | 0.50 |
| 8 | 0.59 | 0.47 |
| 1 | 0.58 | 0.44 |
| 12 | 0.58 | 0.44 |
| 20 | 0.58 | 0.47 |
| 11 | 0.57 | 0.45 |
| 3 | 0.54 | 0.41 |
| 14 | 0.53 | 0.34 |
| 15 | 0.50 | 0.28 |
| 16 | 0.50 | 0.42 |
| 19 | 0.45 | 0.40 |