

Table S3: Comparison (whole length) between EVfold and NiDelta on the benchmark proteins.

| PDB ID | EVfold   |          | NiDelta |          |
|--------|----------|----------|---------|----------|
|        | RMSD (Å) | TM score | RMSD(Å) | TM score |
| 1DMB   | 12.627   | 0.3857   | 6.49    | 0.64     |
| 1E6K   | 4.017    | 0.6477   | 4.21    | 0.64     |
| 1F21   | 4.533    | 0.6210   | 5.47    | 0.56     |
| 1N0S   | 11.632   | 0.3315   | 5.02    | 0.59     |
| 1R9H   | 7.671    | 0.5929   | 3.34    | 0.68     |
| 1RQM   | 9.070    | 0.3506   | 2.12    | 0.80     |
| 1SVN   | 7.977    | 0.7302   | 5.17    | 0.69     |
| 1TVG   | 14.305   | 0.2604   | 4.77    | 0.63     |
| 1ZGG   | 3.672    | 0.7065   | 2.52    | 0.82     |
| 2JSZ   | 17.073   | 0.2987   | 2.38    | 0.83     |
| 2K1S   | 13.173   | 0.3384   | 3.11    | 0.76     |
| 2KPT   | 12.516   | 0.2849   | 2.19    | 0.80     |
| 2KSY   | 10.585   | 0.4033   | 5.24    | 0.65     |
| 2LCG   | 3.910    | 0.7298   | 2.51    | 0.79     |
| 2LTM   | 12.622   | 0.2633   | 3.42    | 0.69     |
| 3MER   | 14.744   | 0.4071   | 4.99    | 0.63     |
| 5P21   | 4.736    | 0.6890   | 2.98    | 0.77     |
| 2LCI*  | –        | –        | 4.08    | 0.68     |

\*EVfold web-server cannot predict the structure of the protein.