**Supplementary file 2. Templates and confidence values in SaPIbov1 Stl repressor models generated by I-Tassera and Phyre2b servers.**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Server** | **Template information** | **PDB code** | **Aligned**  **Residuese** | **Confidencef**  **(%)** | **Identity**  **(%)** |
| Phyre2 | PrgX transcription factor (*E. Coli*) | 2GRM | 14-261 | 99.8 | 12 |
| Lmo0325 transcription factor (*L. monocytogenes*) | 4RYK | 13-260 | 99.8 | 12 |
| Rgg2 transcription factor (*S. dysgalactiae*) | 4YV9 | 14-263 | 99.7 | 12 |
| PlcR transcription factor (*B. thuringiensis*) | 2QFC | 12-261 | 99.7 | 13 |
| HTH-like transcriptional regulator YbaQ (*E. coli*) | 2EBY | 11-96 | 99.6 | 15 |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Server** | **Top threading templates** | **Closest structural analog** | **Top final model** | | |
| **C-scorec** | **TM-scored** | **RMSD (Å)** |
| I-Tasser | 2QFC, 5D50, 3U3W, 2Bnn, 4RYK, 2AWI | 2QFC. PlcR transcription factor (*B. thuringiensis*) | -1.65 | 0.51 ± 0.15 | 9.7 ± 4.6 |

aSee reference (Yang et al., 2015) for details.

bSee reference (Kelley, Mezulis, Yates, Wass, & Sternberg, 2015) for details.

cC-score is a confidence score for estimating the quality of predicted models , typically ranging between -5 and 2, where a higher value signifies a model with a higher confidence.

dTM-score is a scale for measuring the structural similarity between two structures. A TM-score >0.5 indicates a model of correct topology and a TM-score <0.17 means a random similarity.

eAligned residues. Part of protein sequence that is aligned with the template sequence.

fConfidence represents the probability (from 0 to 100) that the match between the query sequence and the corresponding template is a true homology. A match with confidence >90%, generally should indicate that the query sequence adopts the overall fold shown by the template and that the core of the protein is modelled at high accuracy.