**Table S1.** **Amino acid sequences of selected bacterial PmrB for constructing ligand-guided homology models.**

|  |  |  |
| --- | --- | --- |
| **Organisms** | **Accession Number** | **Amino Acid Sequence** |
|  |
| *Klebsiella pneumoniae* | WP\_004886129.1 | MALFATENWTMRHRLLLTIGAILVVCQLISVFWLWHESKEQIQLLVASAIEGHNNQKHVEHEVREAVASLLVPSLLIVGLALYISMLAVRKITRPLSRLQSELESRTPDNLTPIVLSESVPEVTAVTTALNQLVSRLNLTLDRERLFTADVAHELRTPLAGLRLHLELLAKVHGMGVDPLIQRLDQMTTSISQLLQLARVGQSFSAGSYQQVLLLDDVVKPLQDELETMLAERQQRLLLTDVESEAVVSGDATLIRVILRNLVENAHRYSPQGSTIRVSVKAGLMPVMAVEDEGPGIDEAKSGELSKAFVRMDSRYGGIGLGLSIVTRIAQLHDAQFFLHNRQPGPGVRAWVLFPRRGGQNVSTH |  |
| *Escherichia coli* | QIR30685.1 | MRFLRRPISLRQRLILTIGAILLVFELISVFWLWHESTEQIQLFEQALRDNRNNDRHIMREIREAVASLIVPGVFMVSLTLFICYQAVRRITRPLAELQKELEARTADNLTPIAIHSATLEIDAVVSALNDLVSRLTSTLDNERLFTADVAHELRTPLAGVRLHLELLAKTHHIDVAPLVARLDQMMESVSQLLQLARAGQSFSSGNYQHVKLLEDVILPSYDELSTMLDQRQQTLLLPESAADITVQGDATLLRMLLRNLVENAHRYSPQGSNIMIKLQEDGGAVMAVEDEGPGIDESKCGELSKAFVRMDSRYGGIGLGLSIVSRITQLHHGQFFLQNRQETSGTRAWIRLKKDQYVANQI |  |
| *Pseudomonas aeruginosa* | AAG08163.1 | MSRAAVPSVRRRLLVNLLVGFVLCWLSVAALTYHLSLKQVNRLFDDDMVDFGEAALRLLDLATEDQAGEDGSITEIIERSREAIQGLPLLRRESALGYALWRDGQPLLSSLNLPPEITAQGPGFSTVEAQGTHWRVLQLNIDGFQIWISENLIYRQHTMNLLLFYSLFPLLLALPLLGGLVWFGVARGLAPLREVQAEVQQRSARHLQPIAVEAVPLEIRGLIDELNLLLERLRTALEAERRLTSDAAHEIRTPLASLRTHAQVALRSEDPKAHARGLLQVSRSVERISTLMEQILLLARLDGDALLEQFHPVNLATLAEDVLSELARQAIDKDIELSLHQETVYVMGIDLWLKAMVGNLVGNALRYTPAGGQVEIRVENRAQHAVLRVRDNGPGVALEEQQAIFTRFYRSPATSSGEGSGLGLPIVKRIVELHFGSIGLGKGLEGKGLEVQVFLPKTQPDATRPPARGPDSGRSHI |  |
|  |
|  |
| *Acinetobacter baumannii* | ADK46865.1 | MHYSLKKRLIWGTSIFSVILGCILIFSAYKVALQEVDEILDTQMKYLAERTAEHPLKTVSSKFDFHKTYHEEDLFIDIWAYKDQAHLSHHLHLLVPPVEQAGFYSHKTAQGIVRTYVLPLKDYQIQVSQQERVREAFAWELAGSMFIPYLIILPFAIFALAAIIRRGLKPIDDFKNELKERDSEELTPIEVHDYPQELLPTIDEMNRLFERISKAQNEQKQFIADAVHELRTPVTALNLQTKILLSQFPEHESLQNLSKGLARIQHLVTQLLALAKQDVTLSMVEPTGYFQLNDVALNCVEQLVNLAMQKEIDLGFVRNEPIEMHSIEPTVHSIIFNLIDNAIKYTPHQGVINISVYTDPDHYACIQIEDSGAGIDPENYDKVLKRFYRVHHHLEVGSGLGLSIVDRATQRLGGTLTLDKSLELGGLSVLVKLPKVLHLNETRA |  |
|  |
|  |
|  |
|  |