**Table S4.** **Protein-ligand interaction profile of all PmrB models in complex with ATP.**

| **Organisms** | **Moiety** | **Interaction type** | **Residue** | **Interaction site** | **Protein Substructure** |
| --- | --- | --- | --- | --- | --- |
| *Acinetobacter*  *baumannii* | Adenine | Hydrogen bond | A373 | Main chain | Catalytic domain |
| 𝜋-𝜋 stacking | Y345 | Side chain | Catalytic domain |
| Ribose | Hydrogen bond | Y388 | Main chain | Lid-loop |
| V390 | Main chain | Lid-loop |
| Phosphate | Salt bridge | K344 | Side chain | Catalytic domain |
| R389 | Side chain | Catalytic domain |
| Hydrogen bond | G397 | Main chain | Lid-loop |
| S398 | Main chain | Lid-loop |
| G399 | Main chain | Lid-loop |
| N341 | Side chain | Catalytic domain |
| T345 | Side chain | Catalytic domain |
| G401 | Main chain | Catalytic domain |
| *Escherichia*  *coli* | Adenine | Hydrogen bond | P294 | Main chain | Catalytic domain |
| 𝜋-𝜋 stacking | Y268 | Side chain | Catalytic domain |
| Ribose | Hydrogen bond | R310 | Side chain | Lid-loop |
| M311 | Main chain | Lid-loop |
| D312 | Main chain | Lid-loop |
| Y315 | Main chain | Lid-loop |
| Phosphate | Salt bridge | R310 | Side chain | Lid-loop |
| Hydrogen bond | G317 | Main chain | Lid-loop |
| I318 | Main chain | Lid-loop |
| G319 | Main chain | Lid-loop |
| G321 | Main chain | Catalytic domain |
| L322 | Main chain | Catalytic domain |
| N264 | Side chain | Catalytic domain |
| Y268 | Side chain | Catalytic domain |
| *Klebsiella*  *pneumoniae* | Adenine | Hydrogen bond | M312 | Main chain | Lid-loop |
| Y316 | Main chain | Lid-loop |
| 𝜋-𝜋 stacking | Y269 | Side chain | Catalytic domain |
| Ribose | Hydrogen bond | L305 | Main chain | Lid-loop |
| G320 | Main chain | Lid-loop |
| L321 | Main chain | Catalytic domain |
| G322 | Main chain | Catalytic domain |
| L323 | Main chain | Catalytic domain |
| S324 | Main chain | Catalytic domain |
| Phosphate | Hydrogen bond | T189 | Side chain | Dhp domain |
| Q193 | Side chain | Dhp domain |
| I319 | Main chain | Lid-loop |
| L321 | Main chain | Catalytic domain |
| *Pseudomonas*  *aeruginosa* | Adenine | 𝜋-𝜋 stacking | Y367 | Side chain | Catalytic domain |
| Hydrogen bond | D391 | Side chain | Catalytic domain |
| Ribose | Hydrogen bond | S411 | Main chain | Lid-loop |
| T414 | Side chain | Lid-loop |
| Phosphate | Hydrogen bond | S420 | Main chain | Lid-loop |
| G421 | Main chain | Lid-loop |
| L422 | Main chain | Lid-loop |
| G423 | Main chain | Catalytic domain |
| G424 | Main chain | Catalytic domain |
| Q294 | Side chain | Dhp domain |