**S5 Table.** Crystallization states, ATP occupancies, pH and resolution.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | **Divalent Cation** | **Nucleotide State** | **ATP Occ.** | **pH** | **Resolution**(Å) | **PDB ID** |
| *Pf*ActI wt  | Ca\* | ATP\* | 1.00\* | 6.5 | 1.30\* | 4CBU\* |
| Mg | ATP/ADP | 0.79 | 6.0 | 1.24 | 6I4D |
| Mg | ADP | 0 | 6.2 | 1.22 | 6I4E |
| *Pb*ActII wt  | Ca\* | ATP\* | 1.00\* | 6.5 | 2.20\* | 4CBX\* |
| Mg | ADP | 0 | 6.3 | 1.87 | 6I4M |
| F54Y | Ca | ATP | 1.00 | 5.9 | 1.40 | 6I4H |
| Mg† | ATP/ADP† | 0† | 5.9 | 1.90† | 6I4I |
| Mg | ADP | 0 | 5.9 | 1.50 | 6I4J |
| G115A  | Ca | ATP | 0 | 5.9 | 1.83 | 6I4K |
| Mg | ATP/ADP | 0.54 | 5.9 | 1.83 | 6I4L |
| H74Q | Mg | ATP | 0 | 5.8 | 2.00 | 6I4G |
| A272W | Mg | ATP/ADP | 0.32 | 5.8 | 1.50 | 6I4F |

\*Structures reported in ref. 9.

†Crystallized with AlF3