Phosphorus has long been the target of much research, but in recent years the focus has shifted from being limited only to reducing its detrimental environmental impact, to also looking at how it is linked to the global food security. Therefore, the interest in finding novel techniques for phosphorus recovery, as well as improving existing techniques, has increased. In this study we apply a hybrid simulation approach of molecular dynamics and quantum mechanics to investigate the binding modes of phosphate anions by a small intrinsically disordered peptide. Our results confirm that the conformational ensemble of the peptide is significantly changed, or stabilized, by the binding of phosphate anions and that binding does not take place purely as a result of a stable P-loop binding nest, but rather that multiple binding modes may be involved. Such small synthetic peptides capable of binding phosphate could be the starting point of new novel technological approaches toward phosphorus recovery, and they represent an excellent model system for investigating the nature and dynamics of functional de novo designed intrinsically disordered proteins.