Supplementary Information

Structure of Human PIR1, an Atypical Dual Specificity Phosphatase

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Figure S1. The far UV circular dichroism spectrum of PIR1-C152S-core^{FED} recorded from a 6 µM sample of purified protein dissolved in 20 mM sodium phosphate buffer pH 8 and 170 mM NaCl.

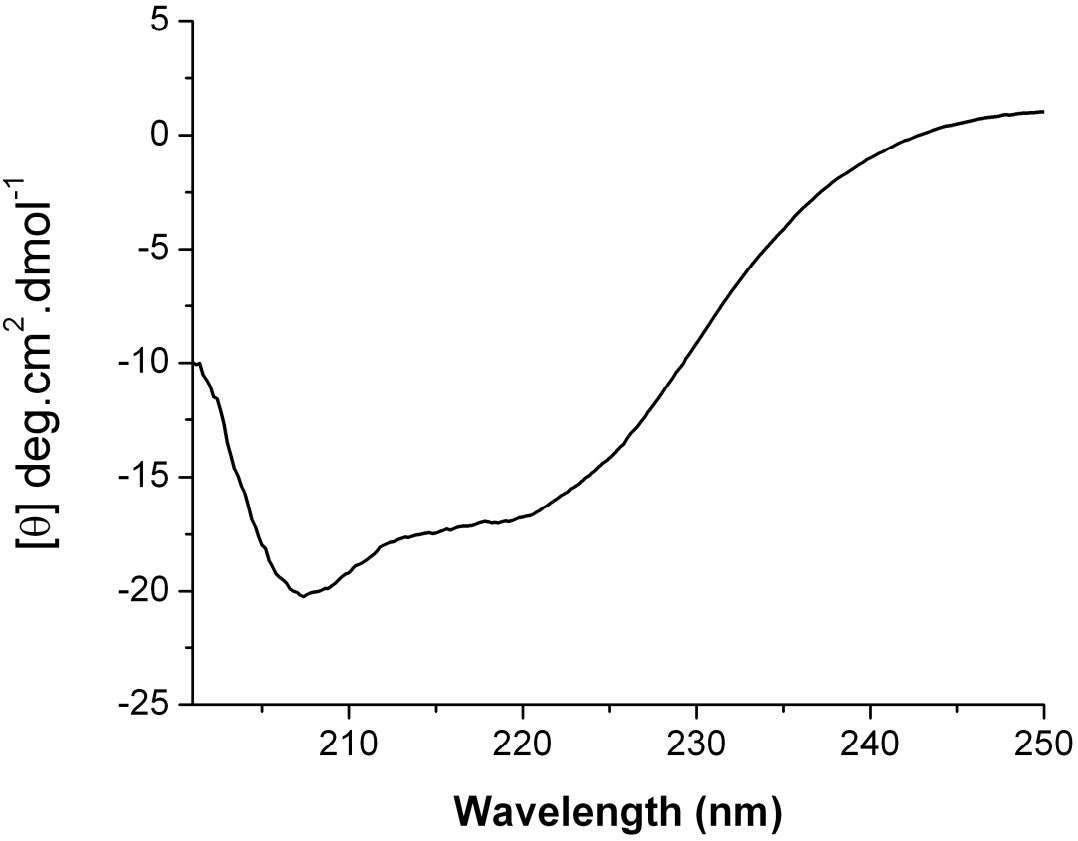


Figure S2. Thermal denaturation of PIR1-C152S-core monitored by measuring temperature-induced CD changes in ellipticity at 222 nm. PIR1-C152S-core unfolded irreversibly with *app*Tm ~57.2 °C.

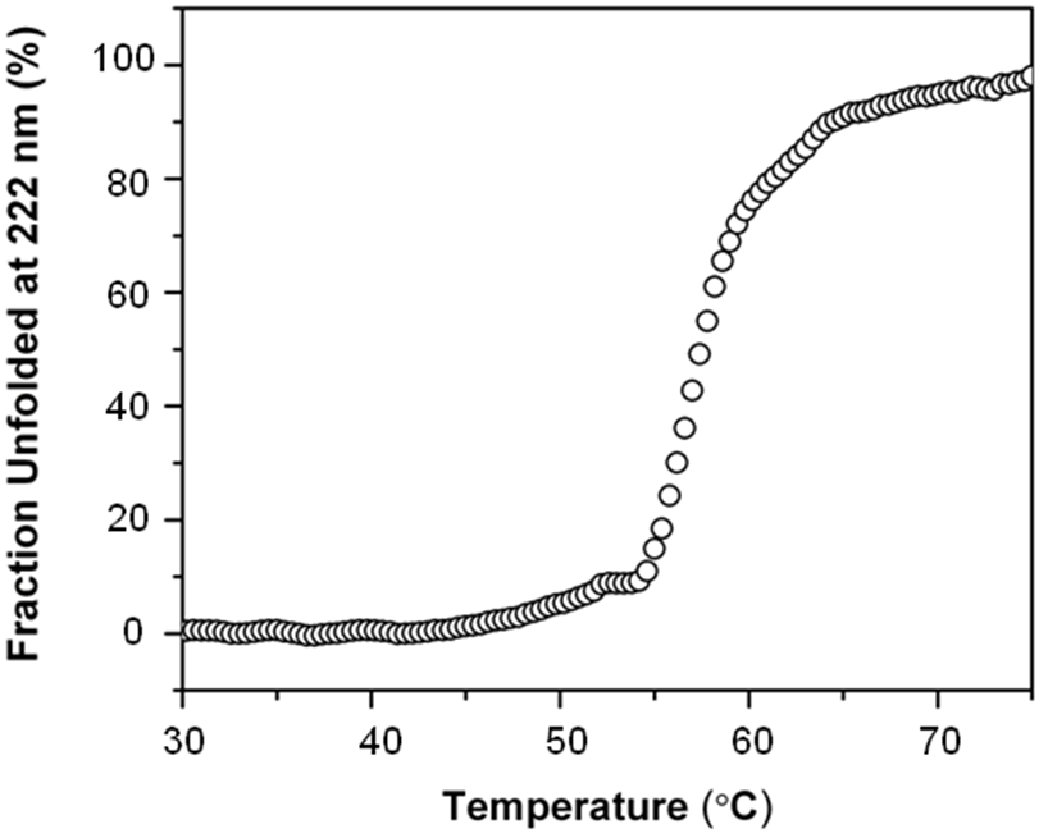


Figure S3. Superimposition of the cubic (gray) and orthorhombic (red) crystal structures of PIR1-C152S-core solved at 1.85Å and 1.20Å resolution, respectively. The rmsd between the two structures is ~0.32 Å. The ribbon diagrams were prepared using the program Pymol (Delano Scientific).

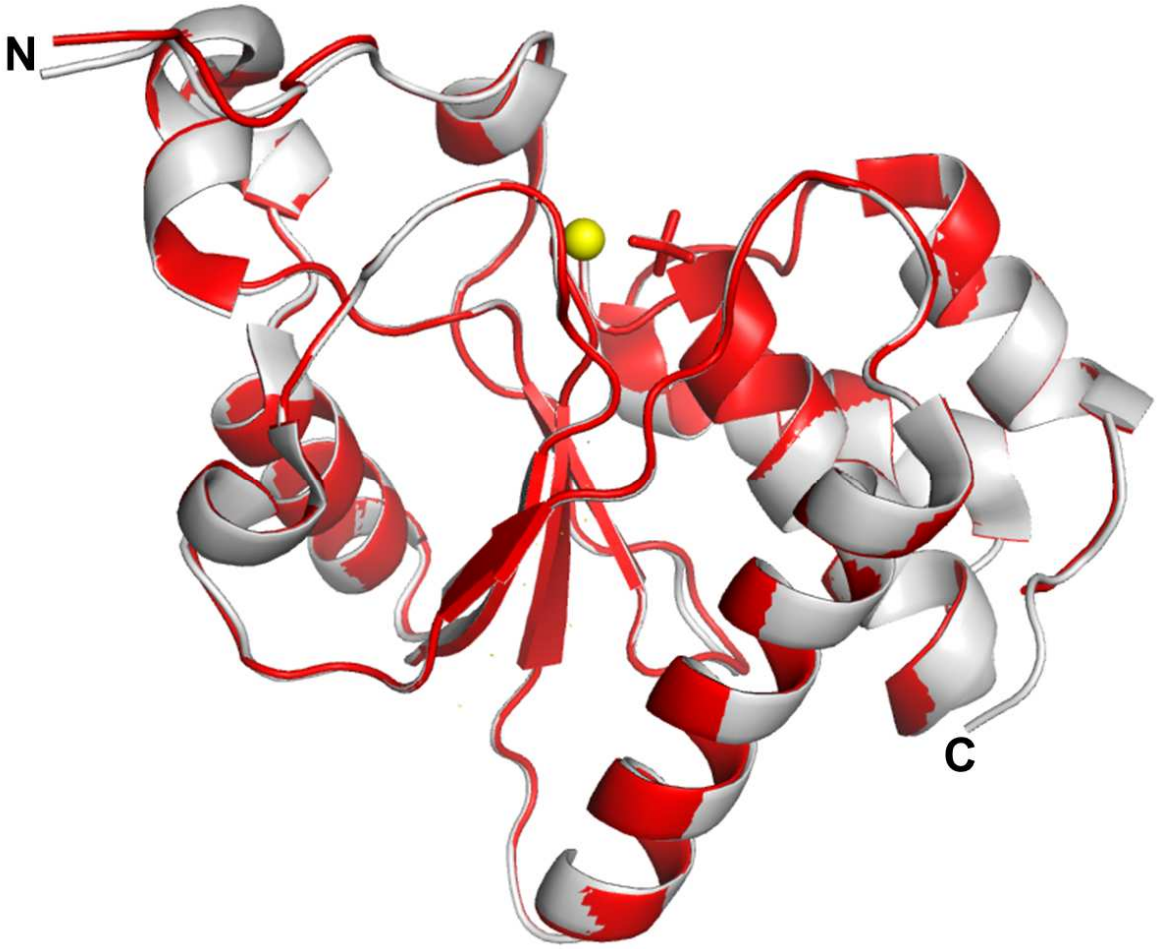
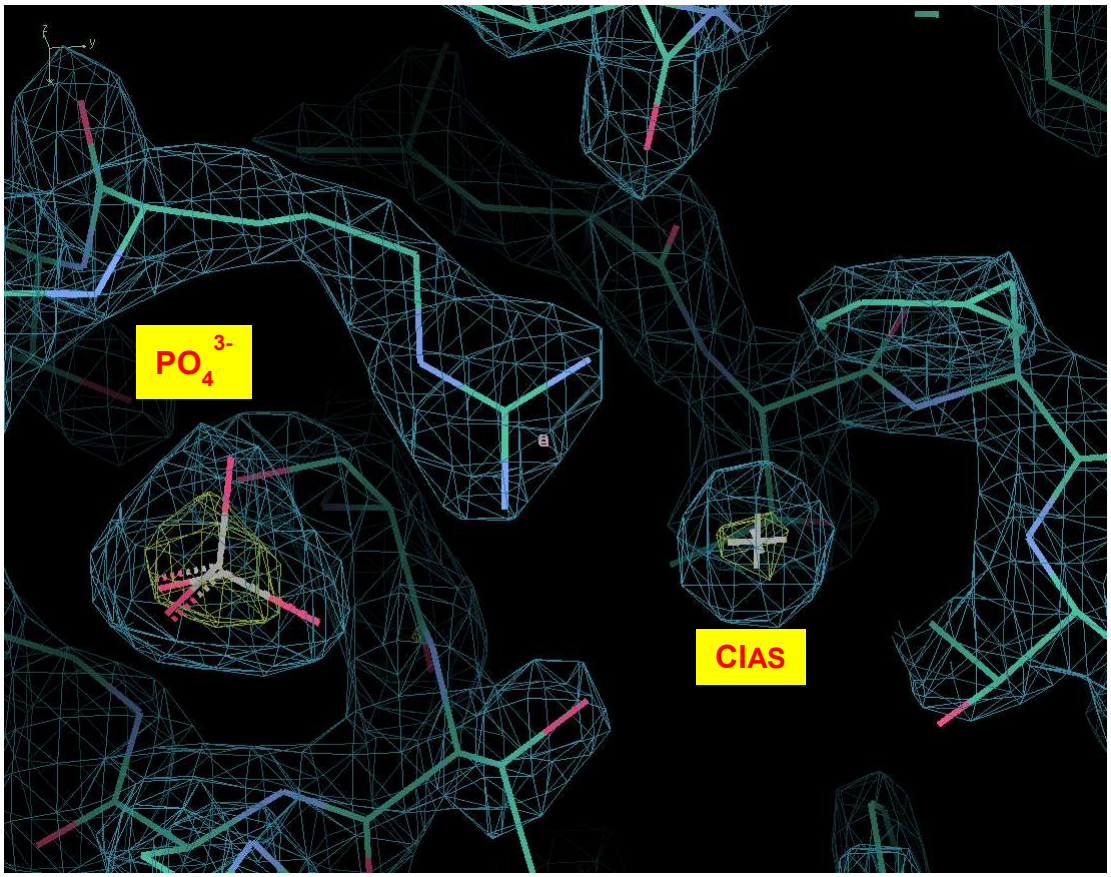


Figure S4. Active site ions visualized in the 2.20 Å crystal structure of PIR1-C152C-core^{FED} crystallized in the presence of ~35mM NaCl. In yellow is an unbiased Fo-Fc difference map contoured at 8σ above background and overlaid to a 2Fo-Fc map (cyan) displayed at 1.5σ. The structure was refined to a Rwork/free of 20.2/25.4% at 2.20 Å resolution. The density was calculated and is displayed using the program Coot (*1*).



REFERENCES

1. Emsley, P., and Cowtan, K. (2004) Coot: model-building tools for molecular graphics, *Acta Crystallogr D Biol Crystallogr 60*, 2126-2132.