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Supporting information for article:

Evaluation of a crystallographic surrogate for kallikrein 5 in the discovery of novel inhibitors for Netherton syndrome

James H. Thorpe, Emma V. Edgar, Kathrine J. Smith, Xiao Q. Lewell, Monika Rella, Gemma V. White, Oxana Polyakova, Pamela Nassau, Ann L. Walker, Duncan S. Holmes, Andrew C. Pearce, Yichen Wang, John Liddle and Alain Hovnanian

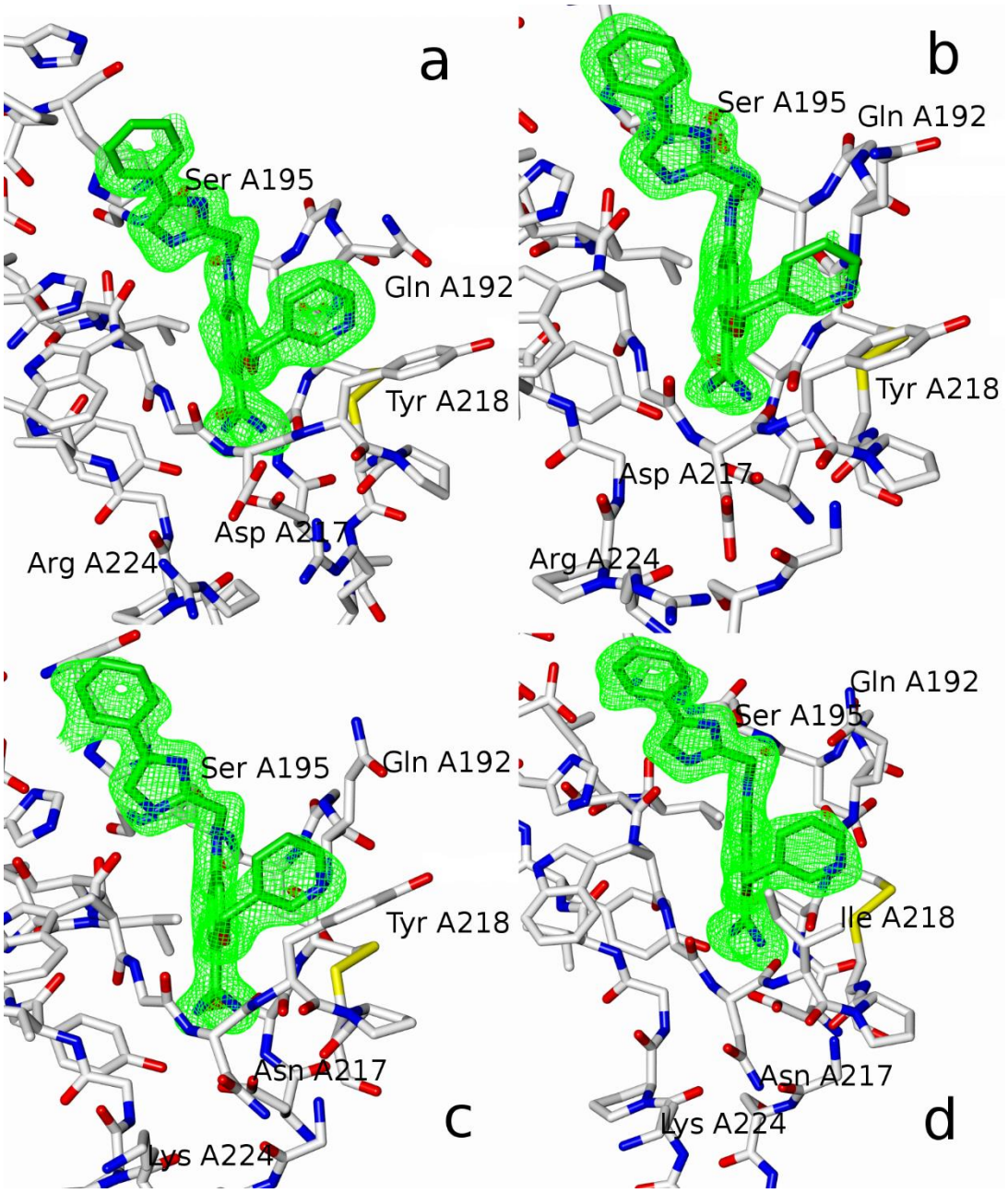

Figure S1 Omit map electron density (green) clipped to GSK144 and scaled at 3σ. Residue labels applied for key residues and mutations (a) KLK5 (b) KLK6TM (N217D I218Y K224R) (c) KLK6SM (I218Y) (d) KLK6WT.

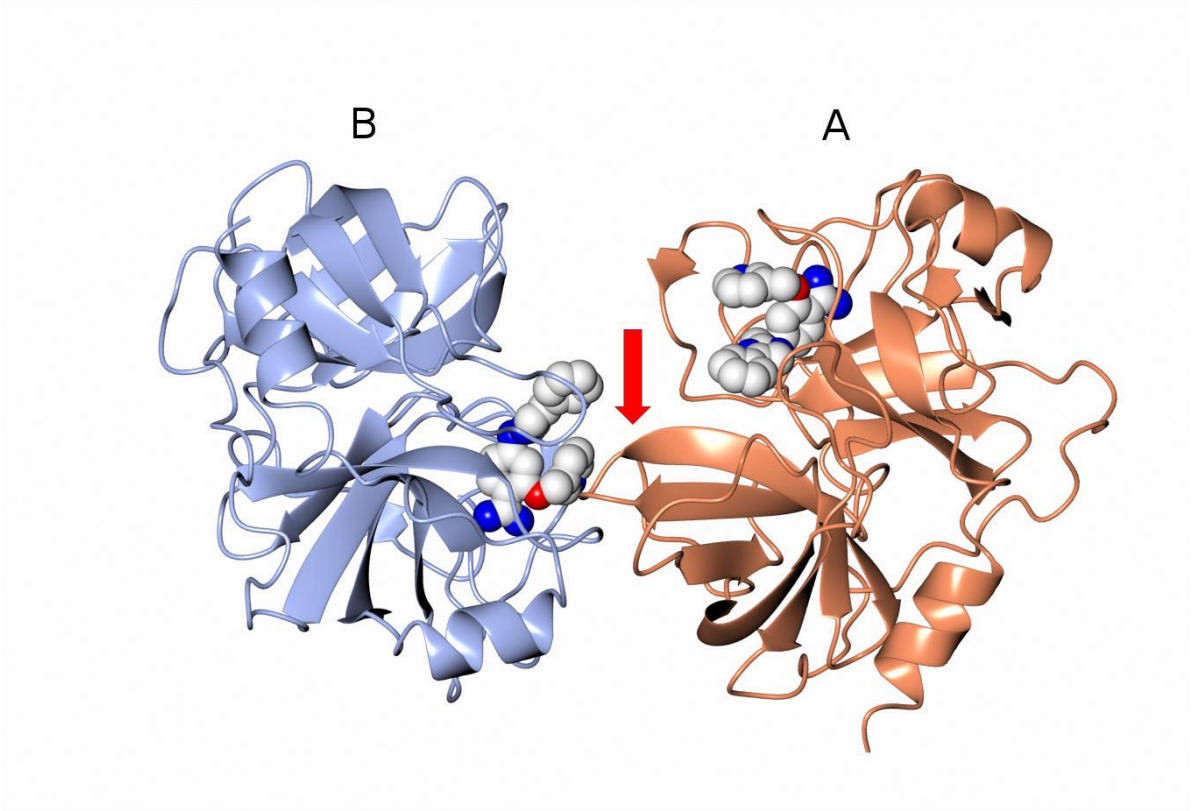

Figure S2 Illustration of the protein chain packing observed for the KLK6 crystal systems where the chain A active site pocket is open to solvent but chain B is influenced by a loop from chain A. Only chain A was therefore utilised when analysing ligand geometry.