

Supplementary material



Fig. 1

Top: Superposition of the hDPPI-Gly-Phe-CHN₂ complex (purple) and 1k3b (yellow).

The C-terminal of the B-chain and the A21-A29 loop are circled.

Bottom: Superposition of the hDPPI-Gly-Phe-CHN₂ complex (purple) and the redetermined native structure (yellow). In both figures, the inhibitor is shown in red sticks and the N-linked carbohydrate is shown in purple and yellow sticks.

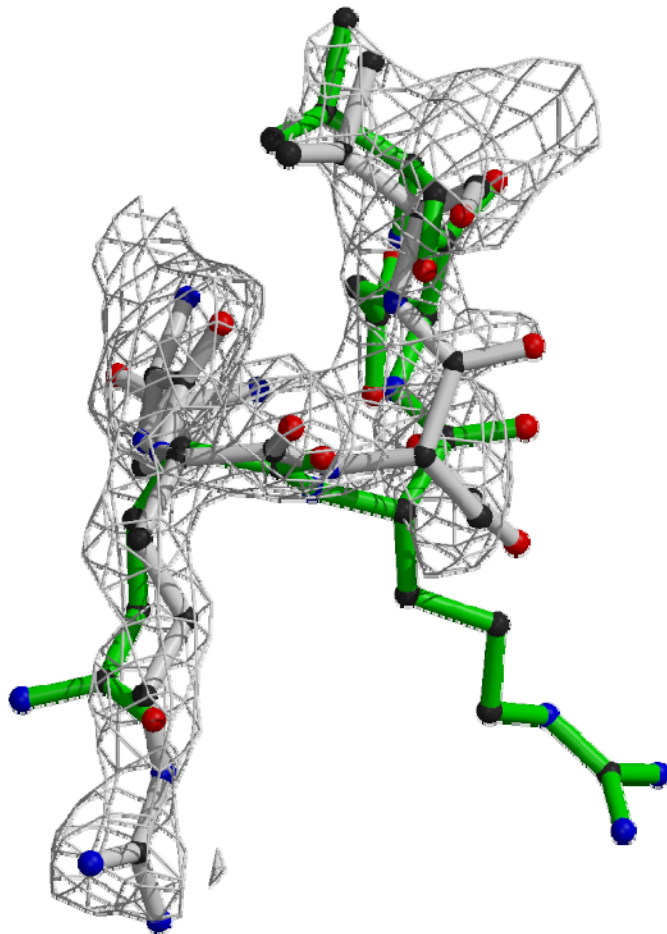


Fig. 2

Fo-Fc electron density map of the A21-A29 loop with the hDPPI-Gly-Phe-CHN₂ structure in gray and the native structure (1k3b) in green.

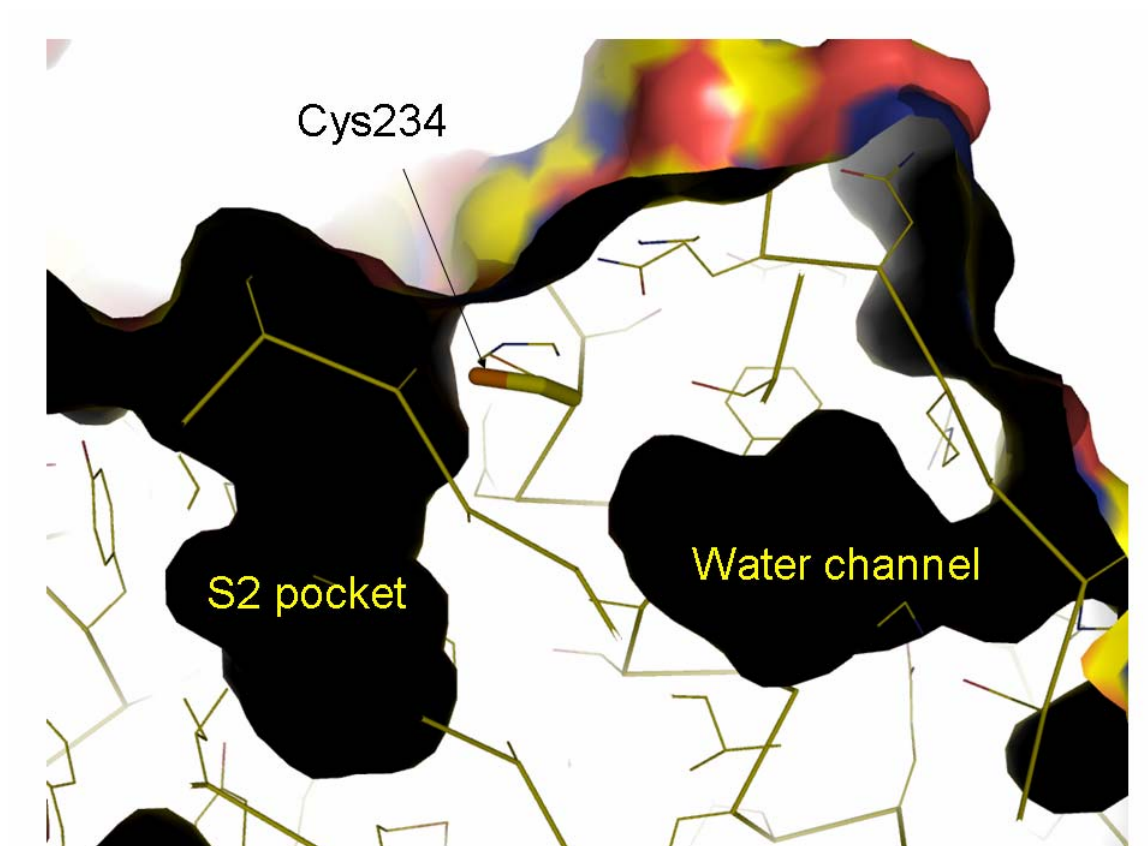


Fig. 3

The native structure of hDPPI near the active site. The surface representation shows the two water filled pockets, which extend into the interior part of the protein structure: the S2 binding pocket and the water channel, which is found behind the catalytic Cys234.