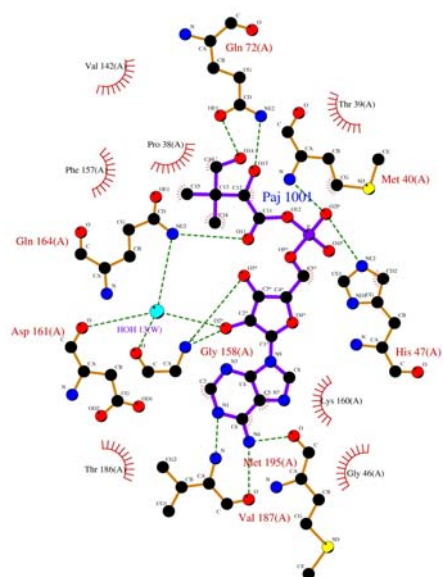


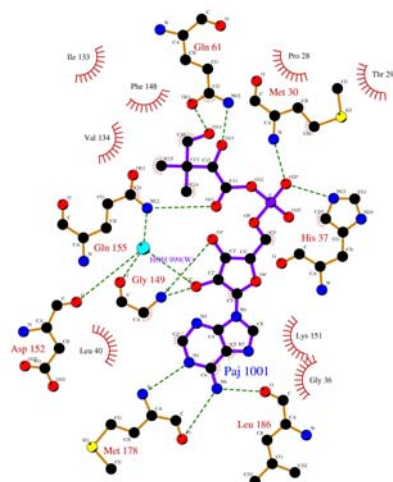
Electronic Supporting Information (ESI)



Key

- Ligand bond
- Non-ligand bond
- Hydrogen bond
- ~~~~~ His 53 Non-ligand residues involved in hydrophobic contact(s)
- Corresponding atoms involved in hydrophobic contact(s)

Diagram of binding interactions made by pantoyl adenylate in the active site of *M. tuberculosis* pantothenate synthetase based on the crystal structure of pantothenate synthetase in complex with pantoyl adenylate **2**. Figure generated using LIGPLOT¹⁵ (from PDB coordinates 1n2h).



Key

- Ligand bond
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- ~~~~~ His 53 Non-ligand residues involved in hydrophobic contact(s)
- Corresponding atoms involved in hydrophobic contact(s)

Diagram of binding interactions made by pantoyl adenylate **2** in the model of the close structure of active site of *E. coli* pantothenate synthetase. Figure generated using LIGPLOT¹⁵.