

### LmrR\_pAF Designer Enzyme with pAF15, H93, and R92 Catalytic Residues



- Forming C1-N15 bond: RS (3.2 Å) → TS1 (1.8 Å) → INT (1.47 Å) → PS (1.28 Å, double bond)
- Breaking C1-OH bond: INT (1.43 Å) → TS2 (2.1 Å) → PS (eliminated as H<sub>2</sub>O)

- pAF15 side chain (N15, aromatic ring)
- Substrate (benzaldehyde, C1, O1, OH groups)

- H93 imidazole ring (proton shuttle)
- R92 guanidinium group (stabilization)