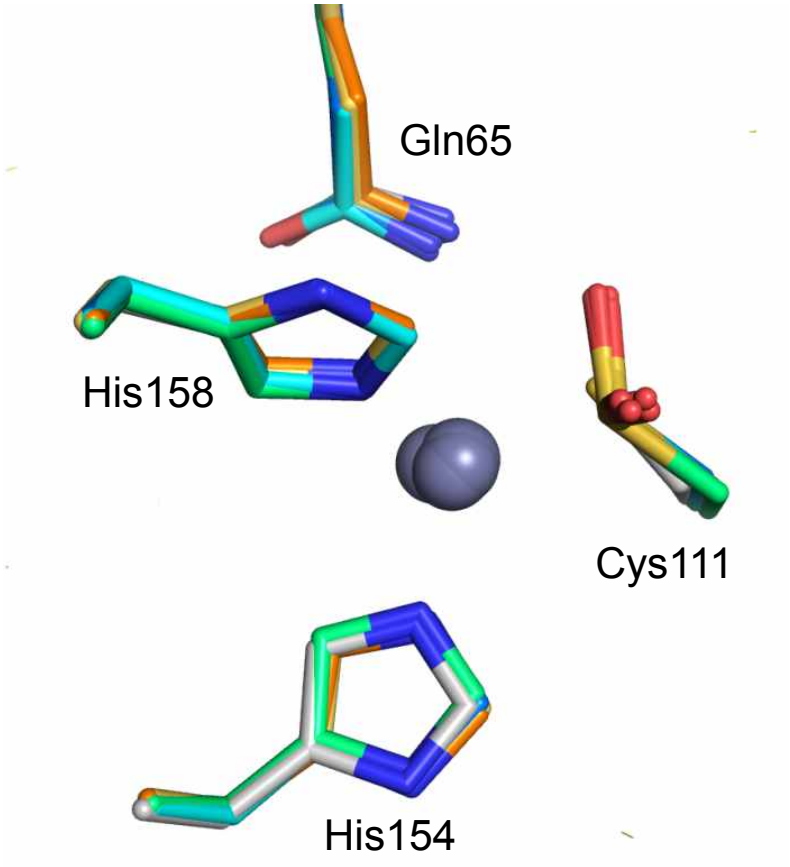
Supplementary Figures

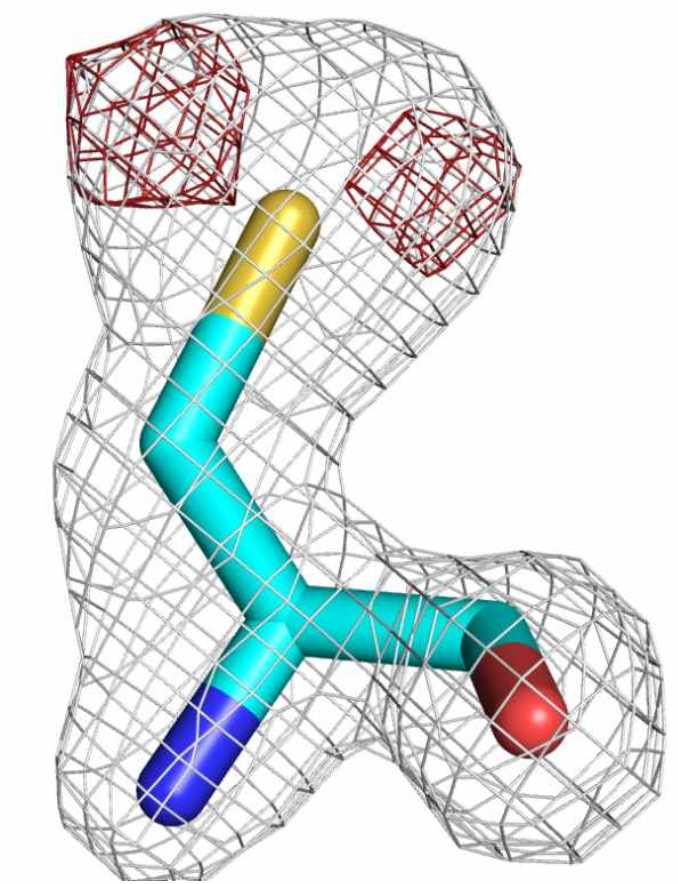
Supplementary Figure S1

(A) Superposition of the metal-coordinating residues (Cys111-SO_2H, Gln65, His154, and His158) in an inhibitor-free structure (PDB code 1LMH) onto the equivalent residues of four inhibitors-bound PDF structures. Structural comparison of Cys111 residues among *S. aureus* PDF structures (containing non-oxidized Cys111 and oxidized Cys111 residues) shows no conformational changes.



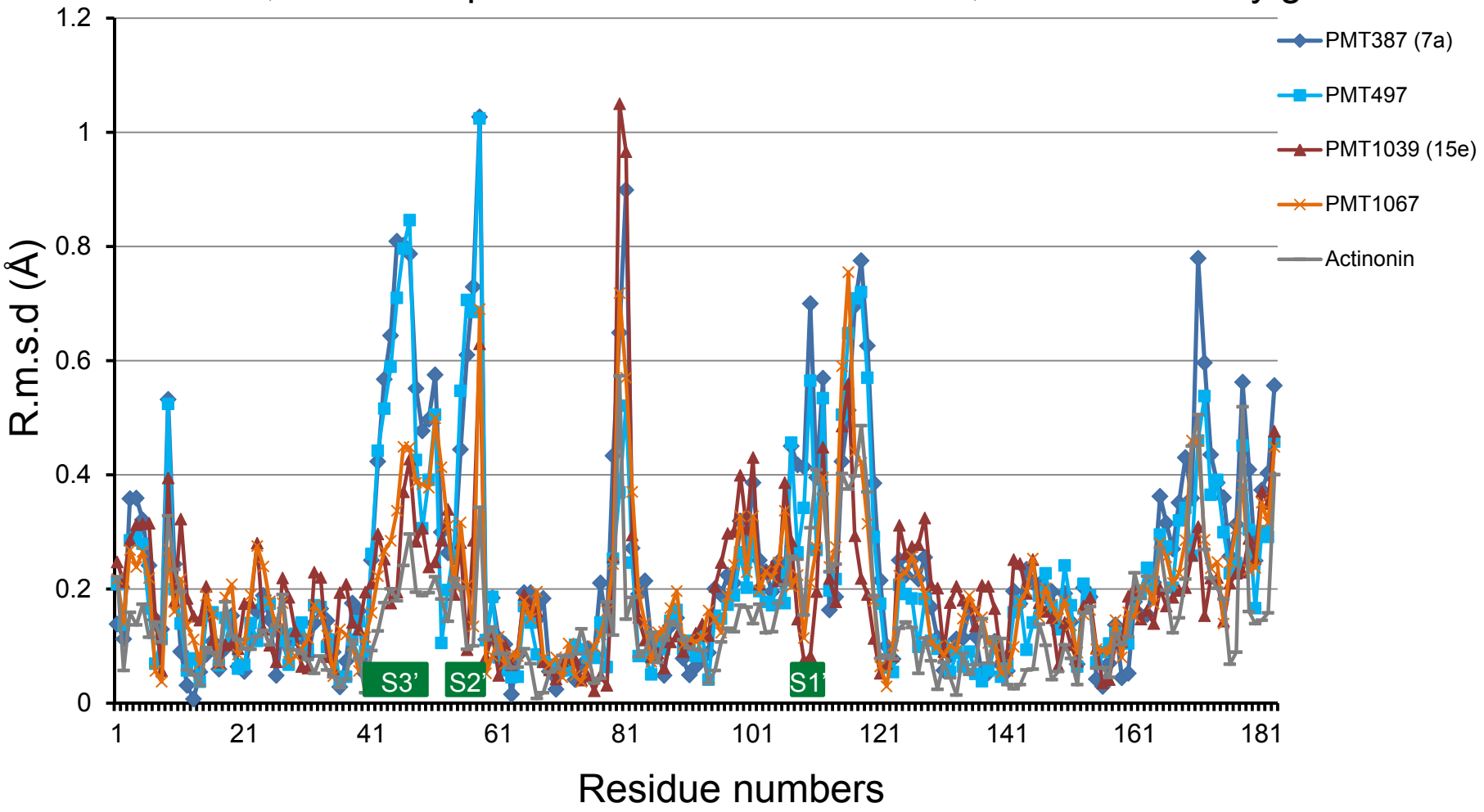
Supplementary Figure S1

(B) *mFo − DFc* electron density map of the oxidized Cys111 (sulfinic acid form) in the PMT387(7a)-bound *S. aureus* PDF. The omit map colored in red (contoured at 4.0σ) was generated with the intact cysteine residue. The omit map colored in grey (contoured at 4.0σ) was generated without the intact cysteine residue.



Supplementary Figure S2

(A) R.m.s.d. plots of the main chain of the four inhibitors [PMT387 (7a), PMT497, PMT1039 (15e), and PMT1067] bound to the *S. aureus* PDF, including an actinonin-bound (PDB code 1Q1Y) PDF structure, are represented by continuous lines. The r.m.s.d were generated compared with the inhibitor-free structure (PDB code 1LMH). The residues, which are positioned into the active site, are indicated by green bars.



Supplementary Figure S2

(B) Average B-factors plots of the four inhibitors [PMT387 (7a), PMT497, PMT1039 (15e), and PMT1067] bound to the *S. aureus* PDF, including an actinonin-bound (PDB code 1Q1Y) PDF structure and an inhibitor-free structure (PDB code 1LMH), are represented by continuous lines. The residues, which are positioned into the active site, are indicated by green bars.