Crystal structure of the wide-spectrum binuclear zinc beta-lactamase from Bacteroides fragilis.

BACKGROUND: The metallo-beta-lactamase from Bacteroides fragilis hydrolyzes a wide range of beta-lactam antibiotics, and therefore, new strategies are urgently needed. Knowledge of the three-dimensional structure will aid in the drug design effort.

RESULTS: The crystal structure of the enzyme has been determined by using multiwavelength anomalous diffraction at the synchrotron. In agreement with the pattern for binuclear zinc binding, the reported structure of the Bacillus cereus enzyme contains only a single zinc.

CONCLUSIONS: Structural analysis indicates that affinity for the penta-coordinated zinc can be modulated by neighboring Asn 193. Consequent to catalysis is stabilized by an oxyanion hole formed by the side chain of the invariant Asn 193 and the tetrahedral zinc.