

## Structure of a Giant Hemoglobin of the Gutless Beard Worm *Oligobranchia mashikoi*

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Pogonophorans and vestimentiferans obtain their nutrition solely from their symbiotic chemoautotrophic sulfur-oxidizing bacteria because they have no mouth or gut. These animals have sulfide-binding 400 kDa and/or 3500 kDa hemoglobin (Hb) which transports oxygen and sulfide simultaneously, and the symbiotic bacteria are supplied with sulfide by these giant Hbs. We have determined for the first time the crystal structure of a 400 kDa vascular Hb from pogonophoran *Oligobranchia mashikoi* at 2.85 Å resolution as an intact oligomeric form. The structure is hollow-spherical, with outer and inner diameters of about 120 Å and 50 Å, respectively, and composed of a total of 24 globins as a dimer of dodecamer. This dodecameric assemblage would be a common unit to both 400 kDa and 3500 kDa Hb. The structure of the mercury derivative used for phasing provides insights into the sulfide-binding mechanism. The mercury compounds bound to all free Cys residues that have been expected as sulfide binding sites. Some of the free Cys residues are surrounded by Phe aromatic rings, and mercury atoms come into contact with these residues in the derivative structure; it is strongly suggested that sulfur atoms bound to these sites could be stabilized by aromatic-electrostatic interactions by the surrounding Phe residues.

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