Supporting Information

Czajkowsky and Shao 10.1073/pnas.0903805106

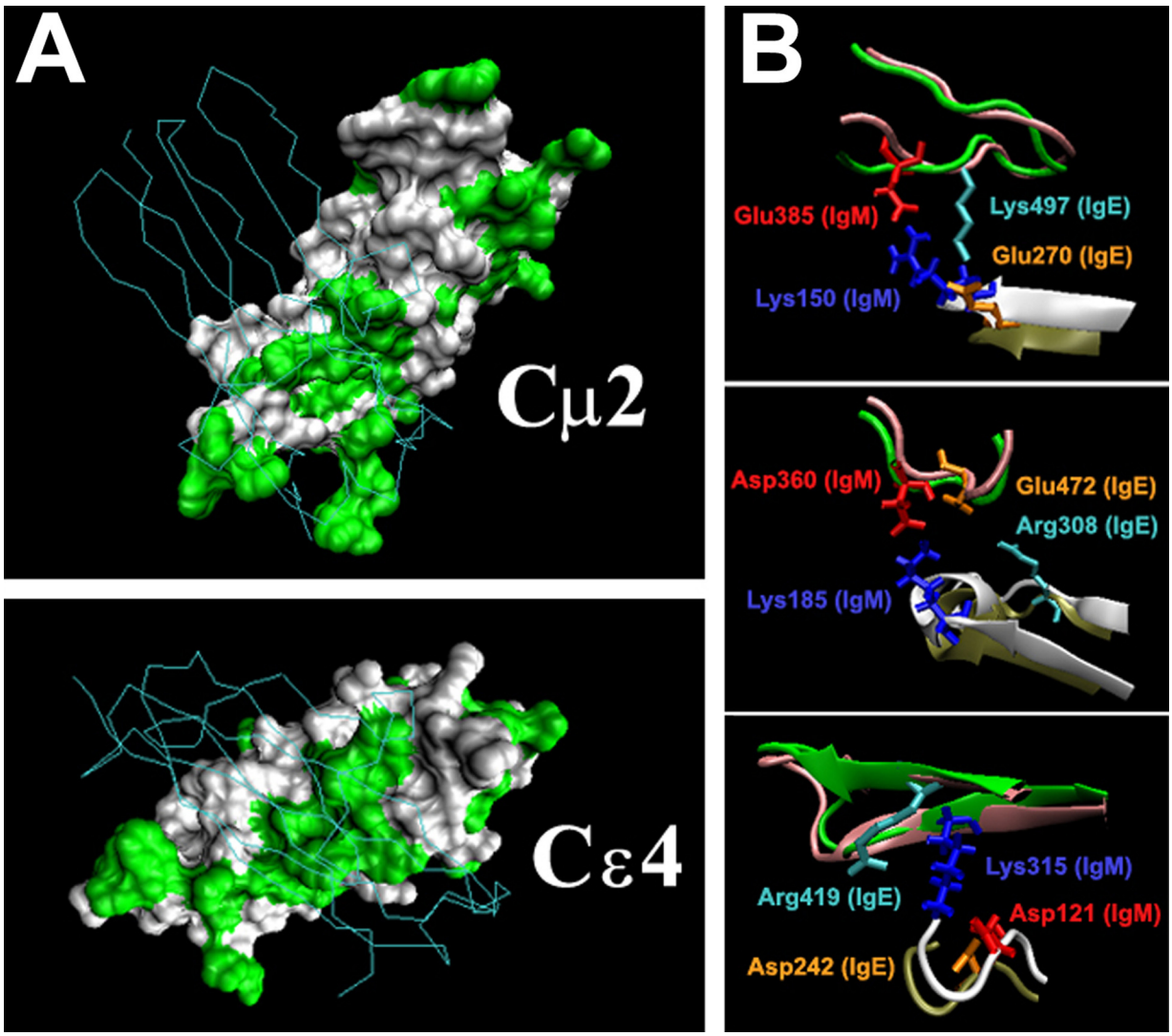

Fig. S1. Unexpected similarities in the domain associations in this Fcμ structure and those observed previously in other interacting Ig domains. (*A*) The Cμ2- Cμ2 interface is predominantly non-polar, as is the case with most Ig domain pairs (1), such as the Cε4-Cε4 pair shown. It is somewhat unexpected here since the Cε2-Cε2 interface is predominantly polar, and so the non-polar character in this structure is not a trivial consequence of the equivalence of the corresponding residues. In each figure, the Cα backbone of one domain is shown as a blue trace and the surface of the other domain is shown with polar residues colored white, hydrophobic residues colored green, and the cysteine residues colored yellow. (*B*) Two of the four salt bridges found in the Cμ2-Cμ3,4 interface link together similar local regions as those in the Cε2-Cε3,4 interface, although none involve conserved residues. A third salt bridge in the Cμ2-Cμ3,4 interface (in the *Bottom*) may also have a correlate to one in the Cε2-Cε3,4 interface, although this salt bridge was not mentioned in the previous work (1). The two IgE heavy chains are colored pink and tan, and the two IgM heavy chains are colored green and white.

1. Wan T, et al. (2002) The crystal structure of IgE Fc reveals an asymmetrically bent conformation. *Nat Immunol* 3:681–686.

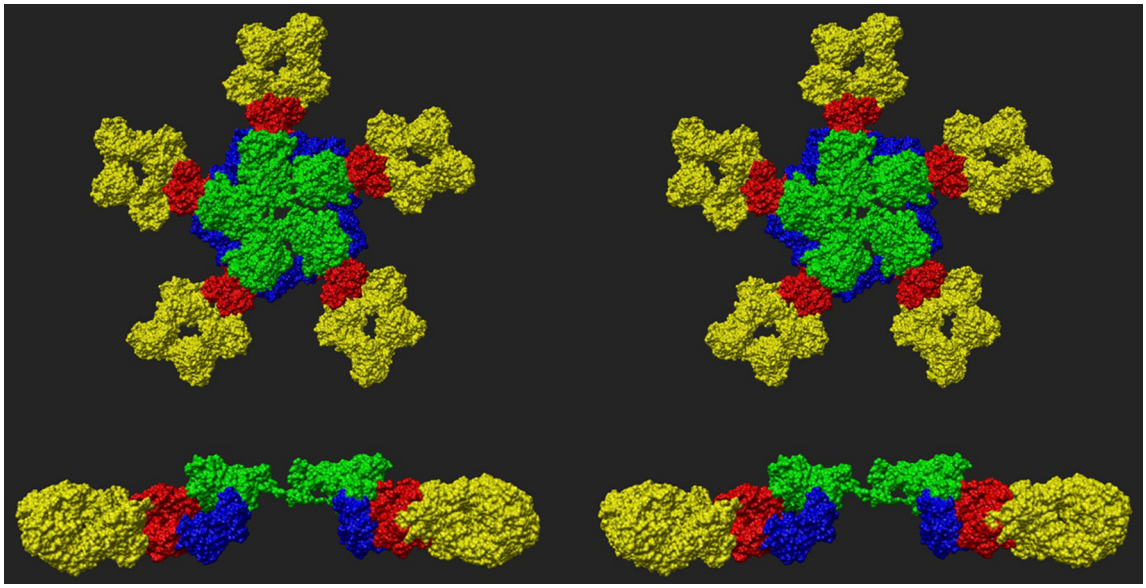

Fig. S2. Stereoview representation of the surface of the IgM pentamer model. In the *Lower*, only two monomers are shown for clarity. The domains of the Fc region are colored as in Fig. 1, and the Fab domains are colored yellow.

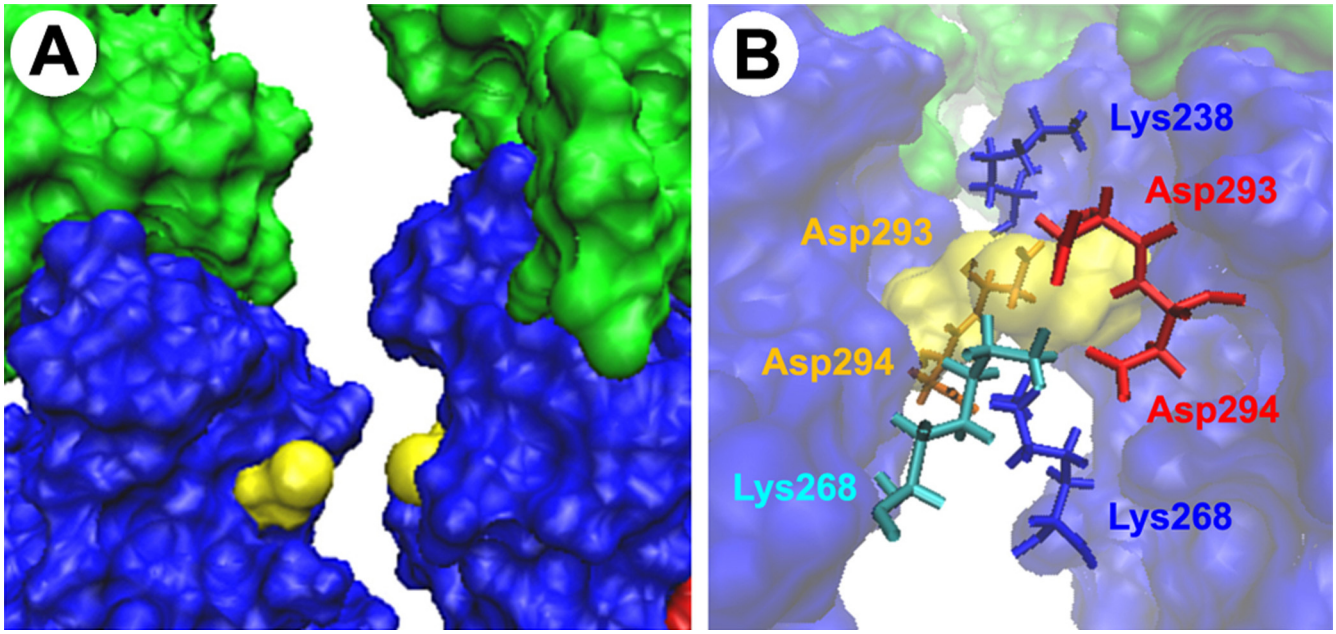

Fig. S3. Structural features of the monomer-monomer interface in the mushroom-shaped IgM complex. (*A*) The interface is characterized by extensive complementarity in the van der Waals surfaces of the two monomers that spans across both Cμ3 and Cμ4 domains. For this figure, the two monomers were separated by 2.5 Å to more clearly show the surface features. The domains and cysteine residues are colored as in Fig. 1. (*B*) There are four salt bridges at this monomer-monomer interface, above and below the disulfide bridge (yellow). The residues involved in these interactions (Lys-238, Lys-268, Asp 293, and Asp-294) are the same in the two monomers, but their relative disposition in this interface is different owing to the asymmetry of the Cμ3 domains in the IgM Fc structure.

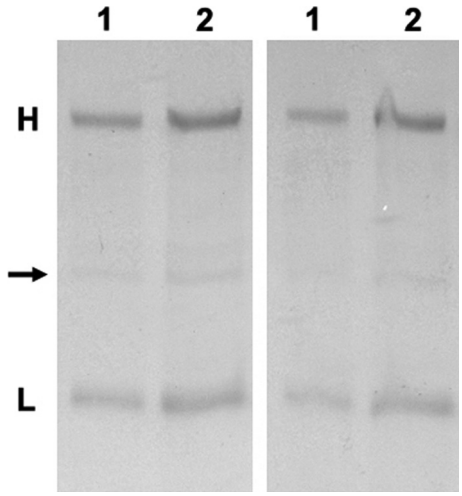

Fig. S4. Confirmation of the quality of the sample by SDS/PAGE in a reducing 4%–20% gradient gel. Labels H and L refer to the bands of the heavy and light chains of IgM, respectively, and the arrow points to a minor band determined to be $<$10% of the heavy chain band. In duplicate, 0.5 μg and 1 μg of the stock IgM solution were added to lanes 1 and 2, respectively.