



STRUCTURAL BIOLOGY
COMMUNICATIONS

Volume 72 (2016)

Supporting information for article:

Structural analysis of a function-associated loop mutant of the substrate-recognition domain of Fbs1 ubiquitin ligase

Kazuya Nishio, Yukiko Yoshida, Keiji Tanaka and Tsunehiro Mizushima

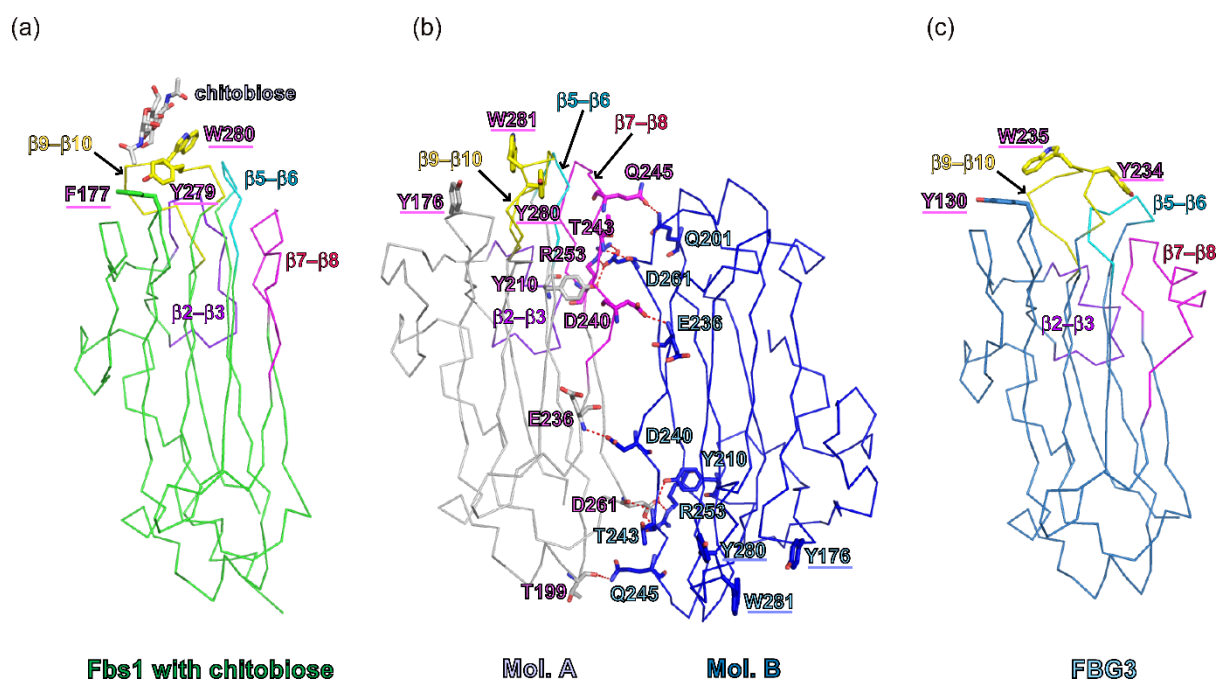


Figure S1 (a) Structure of wild-type Fbs1 SBD with chitobiose (green) (PDB ID: 1UMI) (Mizushima *et al.*, 2004). (b) Structures of Fbs1 SBD loop-mutant 1 Mol. A (gray) and Mol. B (blue) in the asymmetric unit. (c) Structure of FBG3 SBD (sky blue). The hydrogen bonds between Mol. A and Mol. B are indicated as red dashed lines. The residues of hydrogen bonding pairs and the carbohydrate-binding pocket are depicted as stick models. The four loops $\beta 2$ - $\beta 3$, $\beta 5$ - $\beta 6$, $\beta 7$ - $\beta 8$, and $\beta 9$ - $\beta 10$ are colored purple blue, cyan, magenta, and yellow, respectively. Wild-type Fbs1 SBD, Mol A, and FBG3 SBD are shown in the same orientation.

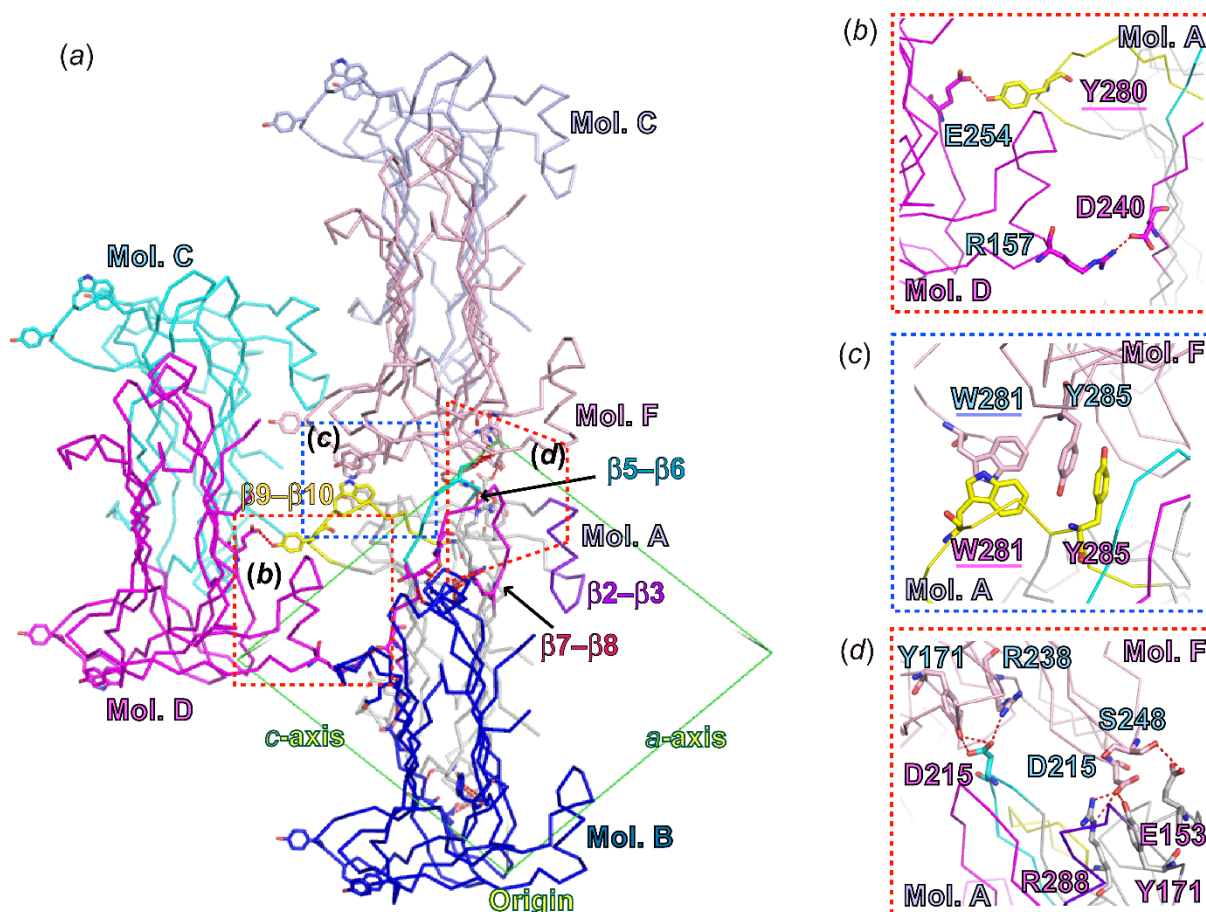


Figure S2 Crystal contacts of Fbs1 SBD loop-mutant 1. (a) The crystal contacts of four loops in the symmetry related molecules from *b*-axis view. Molecules A–F are colored gray, blue, cyan, magenta, light blue, and light pink, respectively. The hydrogen bonds are indicated as red dashed lines. The residues of hydrogen bonding pairs and the carbohydrate-binding pocket are depicted as stick models. The four loops of Mol. A, $\beta 2-\beta 3$, $\beta 5-\beta 6$, $\beta 7-\beta 8$, and $\beta 9-\beta 10$, are colored purple blue, cyan, magenta, and yellow, respectively. (b) Close-up view of the interface between Mol. A and Mol. D. (c) Close-up view of the pi-stacking interaction interface between Mol. A and Mol. F. (d) Close-up view of the interface between Mol. A and Mol. F.