



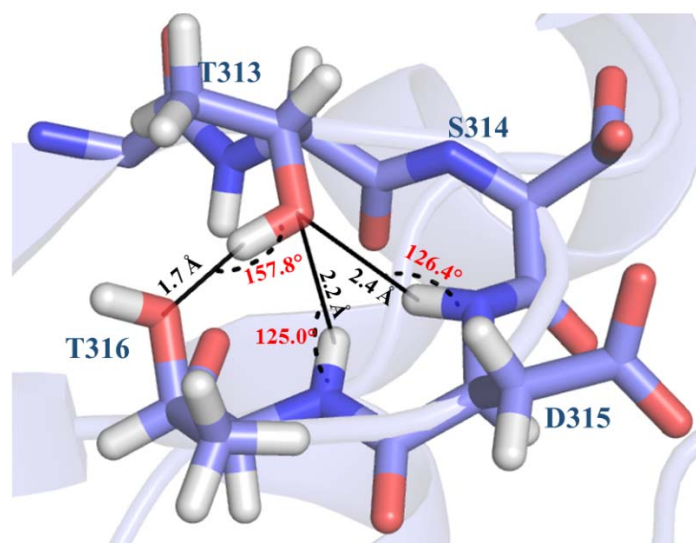
STRUCTURAL BIOLOGY  
COMMUNICATIONS

**Volume 77 (2021)**

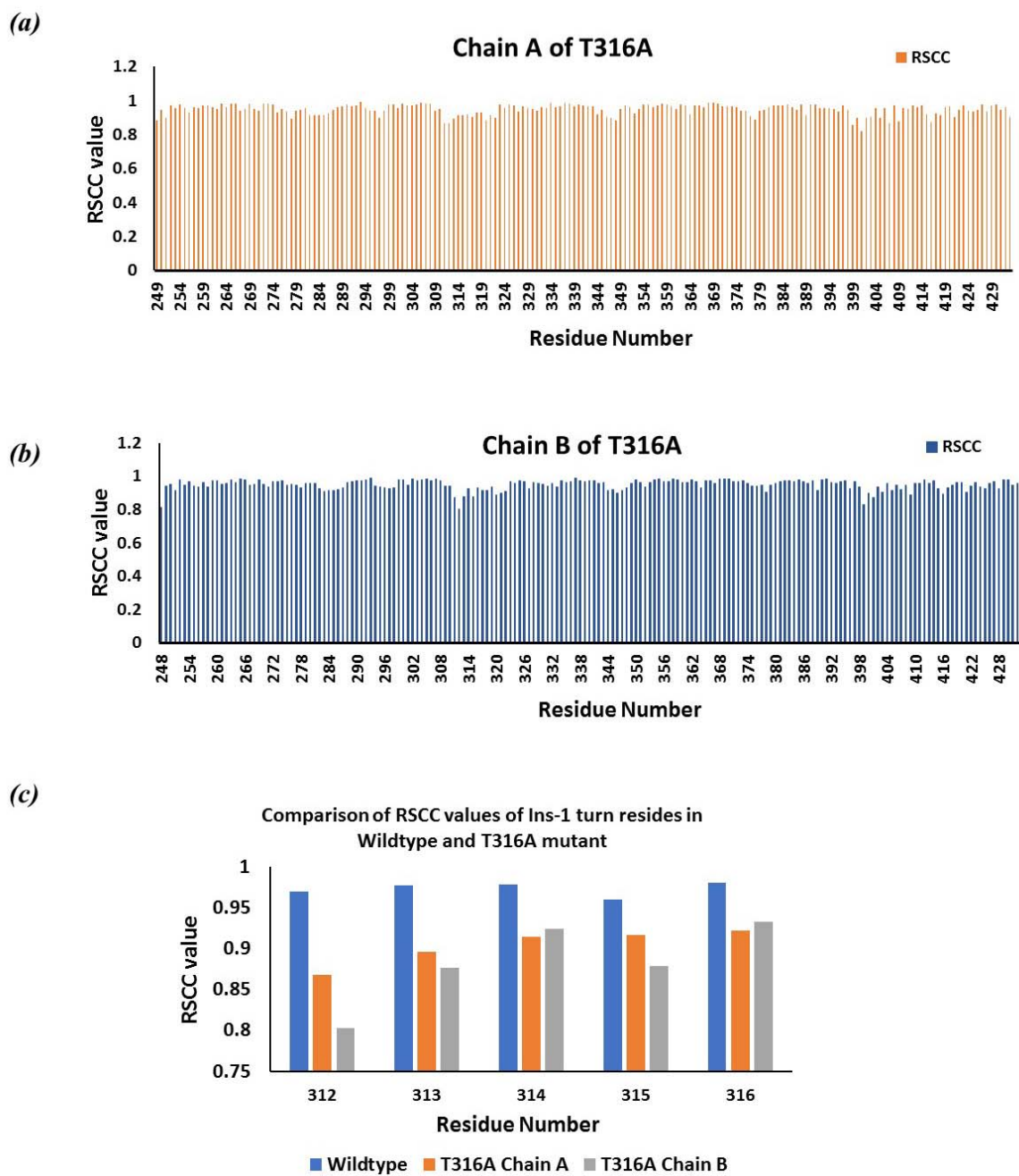
**Supporting information for article:**

**Crystal structure of the Thr316Ala mutant of a yeast JAMM deubiquitinase: implication of active-site loop dynamics in catalysis**

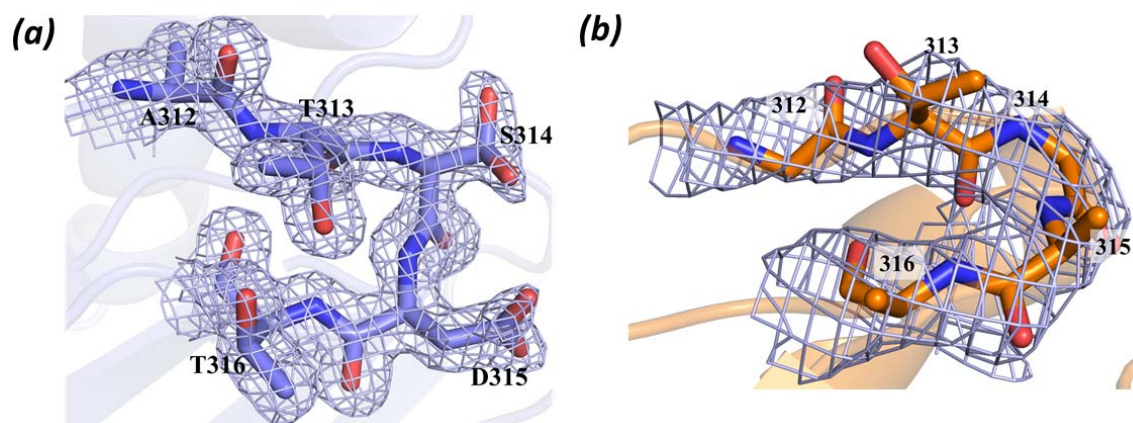
**Rashmi Shrestha and Chittaranjan Das**



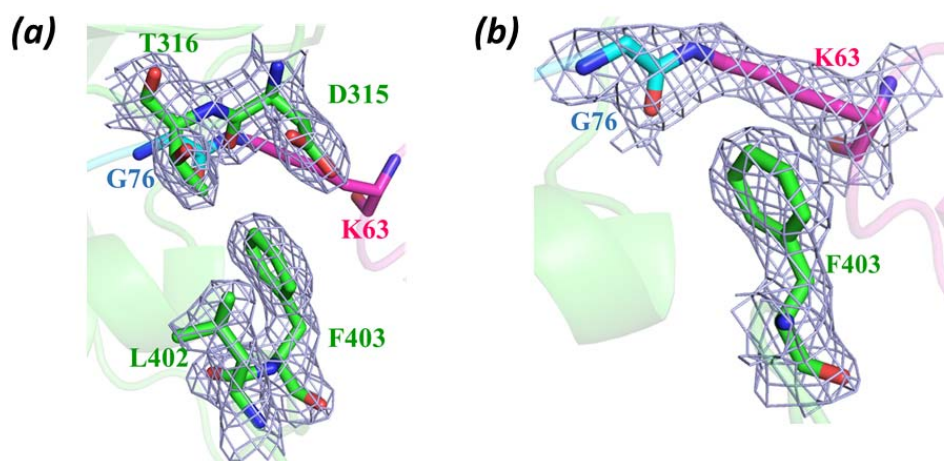
**Figure S1:** Hydrogen bonding geometry formed by Thr313 in Ins-1 turn. The two lone pairs of oxygen and hydrogen in sidechain OH of Thr313 forms hydrogen bonds with two backbone NH groups of Asp315 and Thr316 and oxygen of sidechain OH of Thr316, respectively. The distances between hydrogen bond donor and acceptor in presence of hydrogen are shown in black and the angles are written in red.



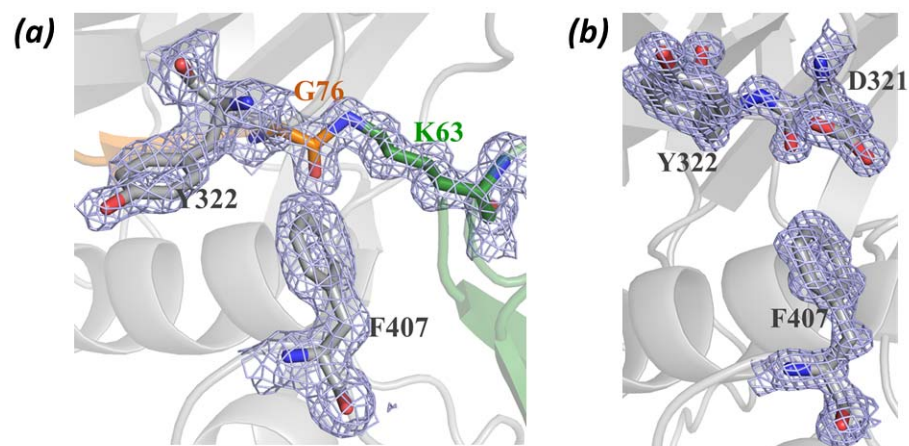
**Figure S2:** Real-space correlation coefficient (RSCC) values of each residue. (a)-(b) Per-residue RSCC values of chain A and chain B of Sst2<sup>T316A</sup> mutant. (c) Comparison of RSCC values of Ins-1 turn residues in wild type Sst2 and T316A mutant.



**Figure S3:** Electron density map of wild type and T316A mutant. (a) The 2Fo-Fc map showing the Ins-1 turn residues in wild type Sst2 (PDB: 4JXE). The map was contoured at 1.2  $\sigma$ . (b) The electron density of Ins-1 turn of Sst2<sup>T316A</sup> mutant, which is rendered from 2Fo-Fc map contoured at 1  $\sigma$ .



**Figure S4:** Electron density map of Sst2 with K63-linked diubiquitin. (a) The electron density enveloping Phe403 of Ins-2, and Asp315 and Thr316 of Ins-1 in K63-linked diubiquitin bound form of Sst2 (PDB: 4NQL). (b) The electron density map of isopeptide bond formed between Lys63 of proximal ubiquitin (magenta) and Gly76 of distal ubiquitin (blue) along with Phe403 (green) of Sst2. These 2Fo-Fc maps are contoured at 1  $\sigma$ .



**Figure S5:** Electron density map of AMSH-LP. (a) The electron density map enveloping residues Phe407 and Tyr322 in K63-linked diubiquitin bound form of AMSH-LP along with Gly76 (orange) and K63 (forest green) of diubiquitin (PDB: 2ZVV). The 2Fo-Fc map is contoured at  $0.8\sigma$ . (b) The electron density map showing Asp321, Tyr322 and the conserved Phe407 in AMSH-LP (PDB: 2ZNR), which is rendered from 2Fo-Fc map contoured at  $2\sigma$ . AMSH-LP in both (a) and (b) are shown in gray.