

Supplementary information

Activation and selectivity of OTUB-1 and OTUB-2 deubiquitinylases

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OTUB1      MAAEEPQQQKQEPLGSDSEGVNCLAYDEAIMAQQDRIQQEIAVQNPLVSEERLELSVLYKE 60
OTUB2      -----MSETSFNLISEKCDILSILR- 20
           .. *:*:*: :: : :

OTUB1      YAEDDNIYQQKIKDLHKKYSYIRKTRPDGNCIFYRAFGFSLHLEALLDDSKELQRFKAVSAK 120
OTUB2      DHPENRIYRRKIEELSKRFTAIRKTKGDGNCIFYRALGYSYLELLGKSREIFKFKERVLQ 80
           : :.*:*:*:*:* *:*:*: *****:*:*:*:*:*..*:*:*: ** :

OTUB1      SKEDLVSQGFTEFTIEDFHNTFMDLIEQVEKQTSVADLLASFNDQSTSDYLVVYLRLLTS 180
OTUB2      TPNDLLAAGFEEHKFRNFFNAFYVVELVEKDGSVSLLKVFNDQSASDHIVQFLRLLTS 140
           : :*:*:*: ** *..*:*:*: ::* *****: **:.** *****:*:*:*:*****

OTUB1      GYLQRESKFFFEHFIEGGRTVKEFCQQEVEPMCKESDHIHIALAQAQSVSIQVEYMDRGE 240
OTUB2      AFIRNRADFFRHFIDEEMDIKDFCTHEVEPMATECDHIQITALSQALSIALQVEYVDEMD 200
           : :*:*:*:*:*:*: :*:* ** :*****..*.*:*:* *:*:*:*:*:*:*:*:*:*:

OTUB1      GGTTPHIFPEGSEPKVYLLYRPGHYDILYK---- 271
OTUB2      T-ALNHHVFPEAATPSVYLLYKTSHYNILYAADKH 234
           : * *:*:*:*:*: *..*****: .**:*:*

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Figure S1: Sequence alignment of OTUB1 and OTUB2. The symbols “*, :, .” represents fully conserved, strongly similar and weakly similar properties, respectively.

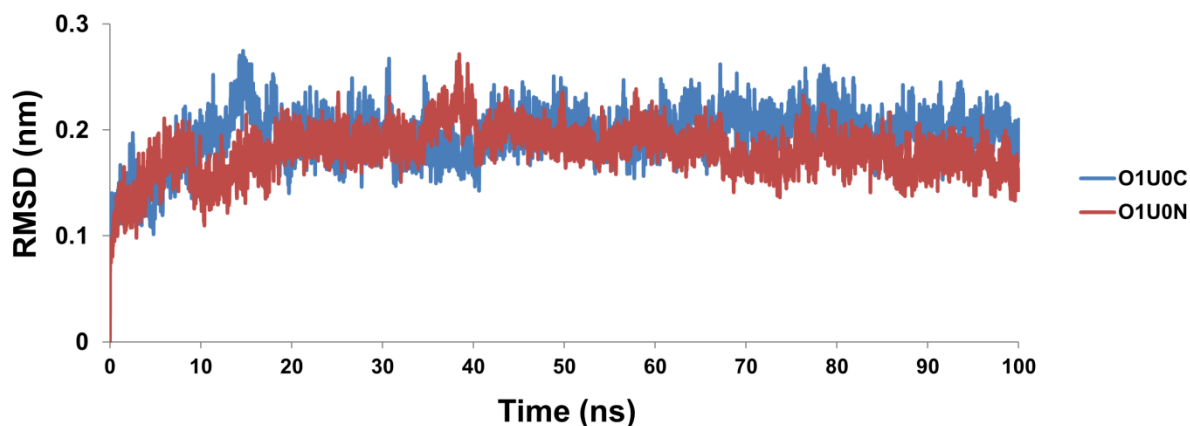


Figure S2: RMSD in nm (Cα) plot of ubiquitin-free OTUB1 in charged O1U0C and neutral O1U0N protonation states of active site residues.

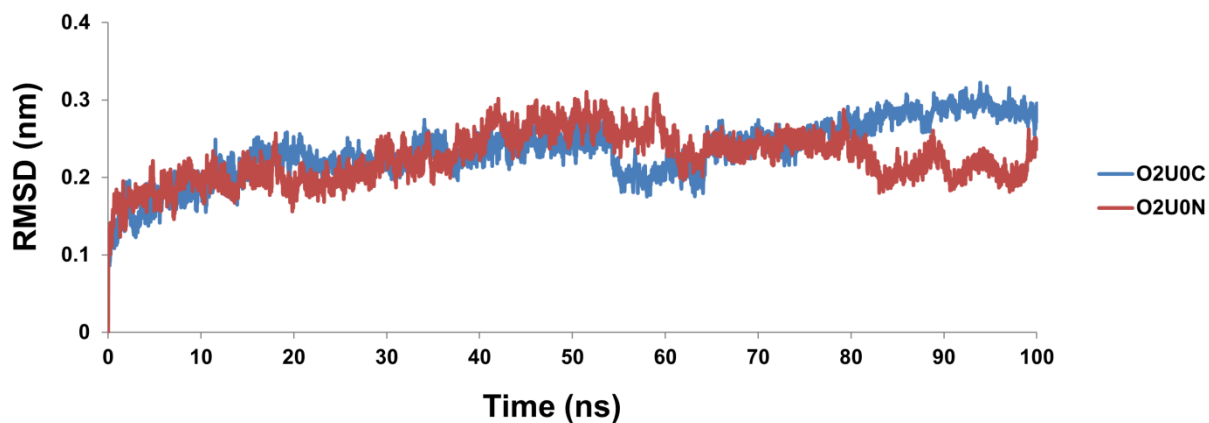


Figure S3: RMSD in nm ($C\alpha$) plot of ubiquitin-free OTUB2 in charged O2U0C and neutral O2U0N protonation states of active site residues.

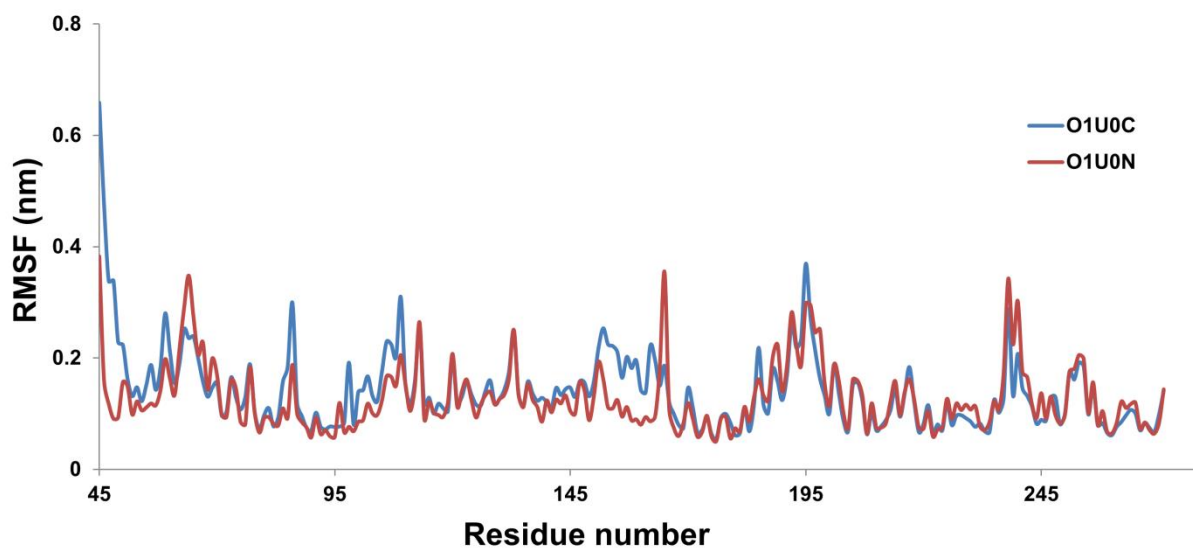


Figure S4: RMSF in nm of amino acid residues of the ubiquitin-free OTUB1 protein conformation in charged O1U0C and neutral O1U0N states of active site residues.

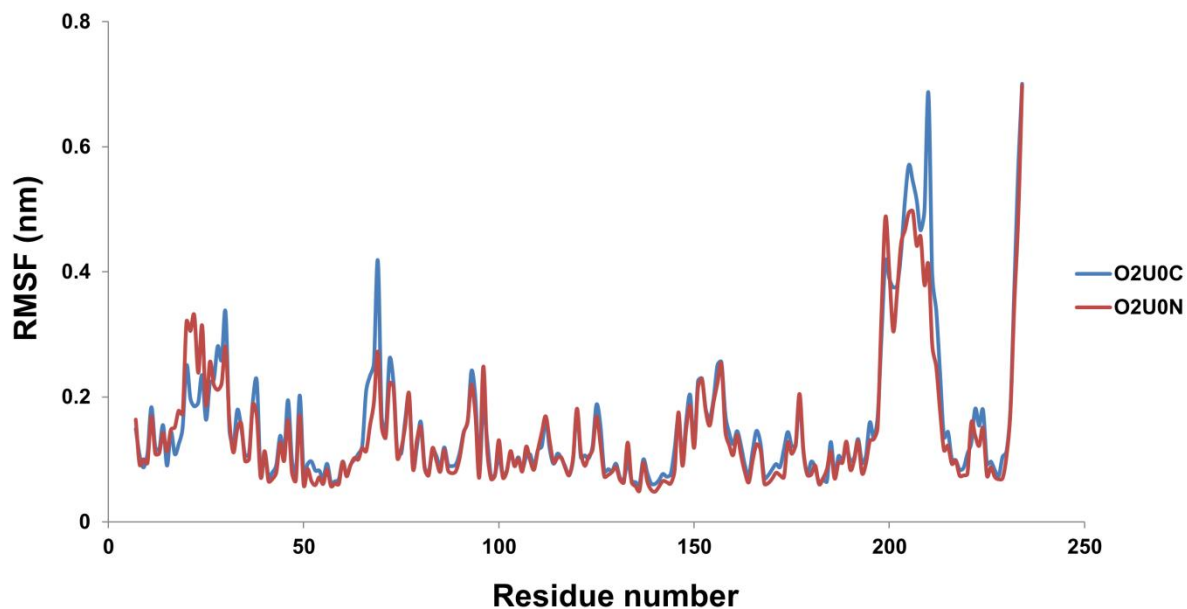


Figure S5: RMSF in nm of amino acid residues of the ubiquitin-free OTUB2 protein conformation in charged O2U0C and neutral O2U0N states of active site residues.

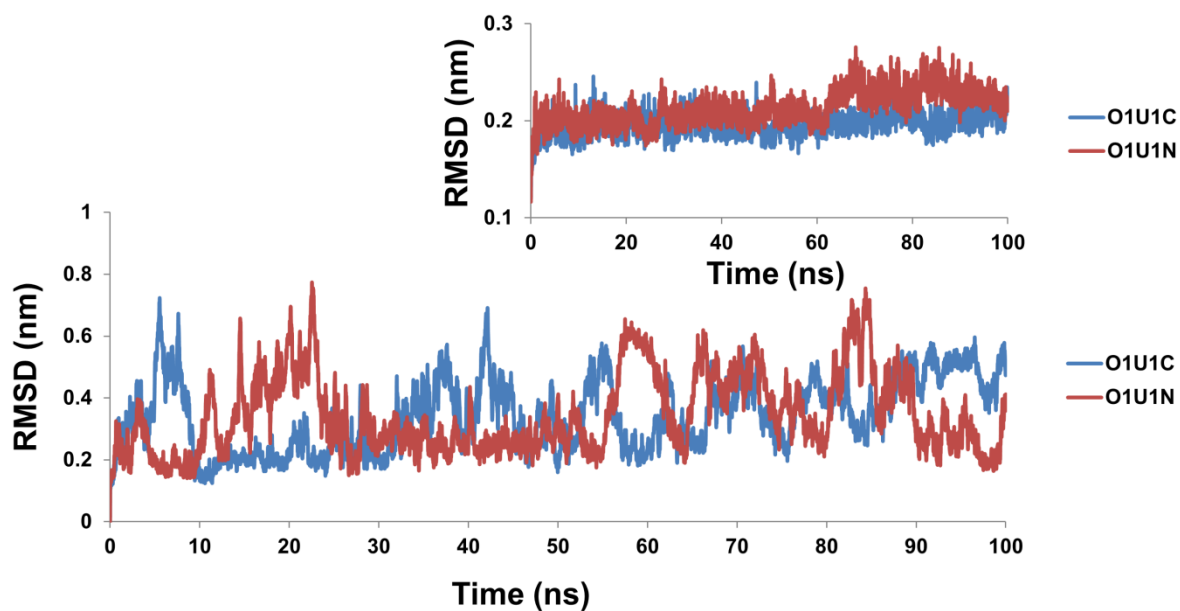


Figure S6: RMSD in nm ($C\alpha$) plot of ubiquitin-bound OTUB1 protein conformation in charged states O1U1C and O1U1N. The inset figure shows the RMSD in nm ($C\alpha$) plot of the holo OTUB1 without N-terminal residues (1-21 amino acids).

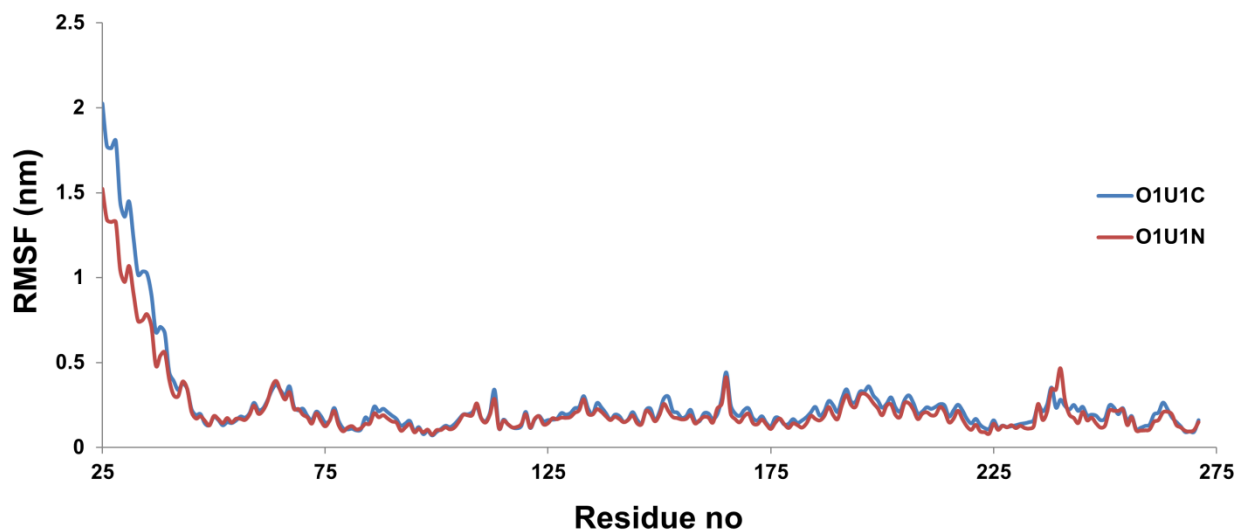


Figure S7: RMSF in nm of amino acid residues of the ubiquitin-bound protein conformation OTUB1 in charged O1U1C and neutral O1U1N protonation states of active site residues.

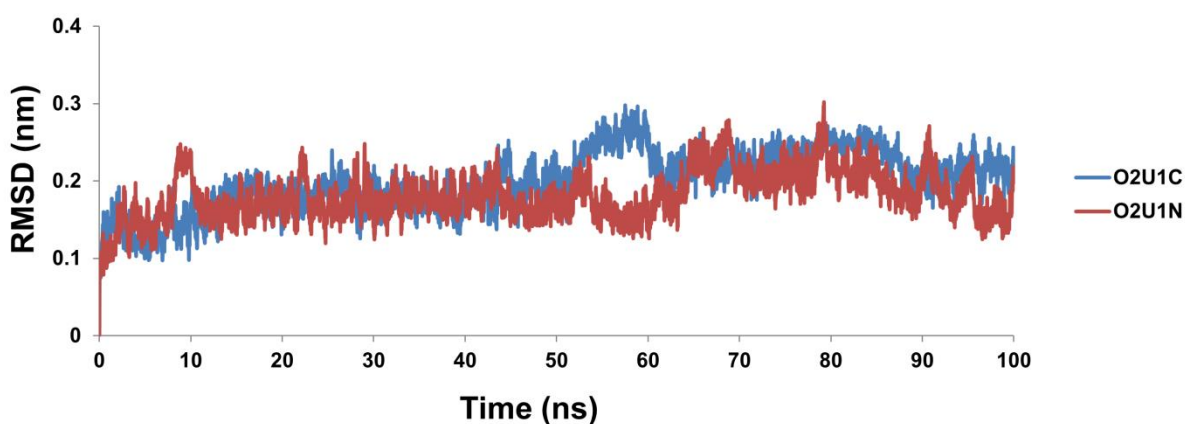


Figure S8: RMSF in nm of amino acid residues of the ubiquitin-bound protein conformation OTUB2 in charged O2U1C and neutral O2U1N protonation states of active site residues.

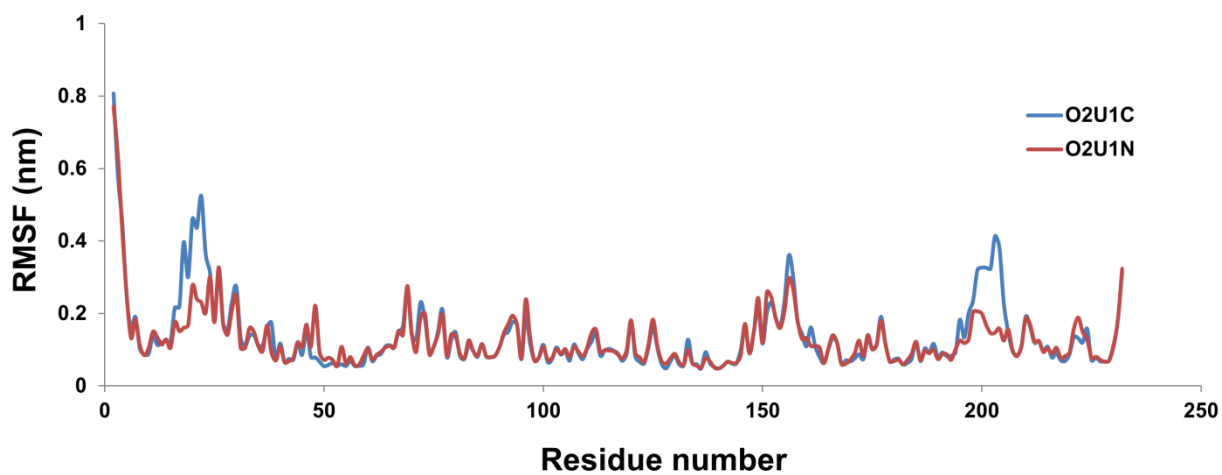


Figure S9: RMSF in nm of amino acid residues of ubiquitin-bound OTUB2 conformation in charged O2U1C and neutral O2U1N states of active site residues.