

Supplementary Information for

Role of the D1-D2 Linker of Human VCP/p97 in the Asymmetry and ATPase Activity of the D1-domain

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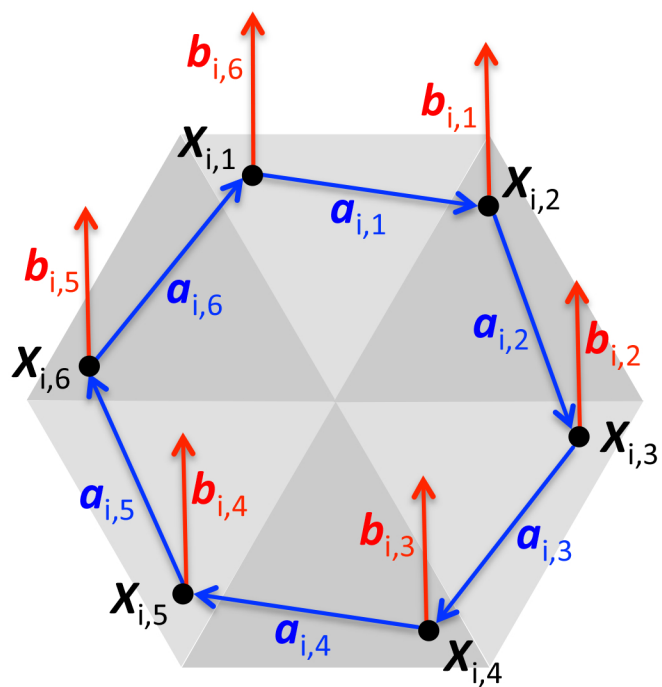
Supplemental Information

Figure S1. Schematic drawing of vectors defined for the calculation of asymmetric index. Symmetric objects such as the six subunits of p97 are represented by shaded triangles. Atom i ($i = 1, 2, \dots, N$), from j^{th} subunit ($j = 1, \dots, 6$) is represented by a dot labeled with $x_{i,j}$ in black color. Vectors drawn between pairs of neighboring atoms are shown as blue arrows labeled with $a_{i,j}$. Cross vectors constructed from neighboring vectors are shown as red arrows labeled with $b_{i,j}$. The asymmetric index (Asym Index) is defined as the averaged angle in degree ($^{\circ}$) among pairs of cross vectors. For a perfect, proper hexamer, in which all cross vectors are parallel to each other, the Asym Index is zero.

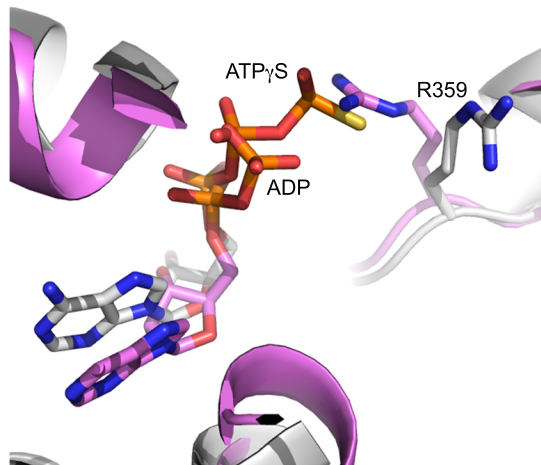
Figure S2. Side-chain conformations of the *in trans* Arg-finger residue R359 in structures of N-D1 p97 bound with either ADP or ATP γ S Structures of wild-type $^{\text{ND1}}\text{p97}^{\text{Shrt}}$ bound with ADP (PDB:1E32) colored in magenta and R155H $^{\text{ND1}}\text{p97}^{\text{Lng}}$ bound with ATP γ S (PDB: 4KO8) in gray are superposed based on the D1-domain. Side-chains of Arg-finger residue R359 and the bound nucleotides are shown in stick representations.

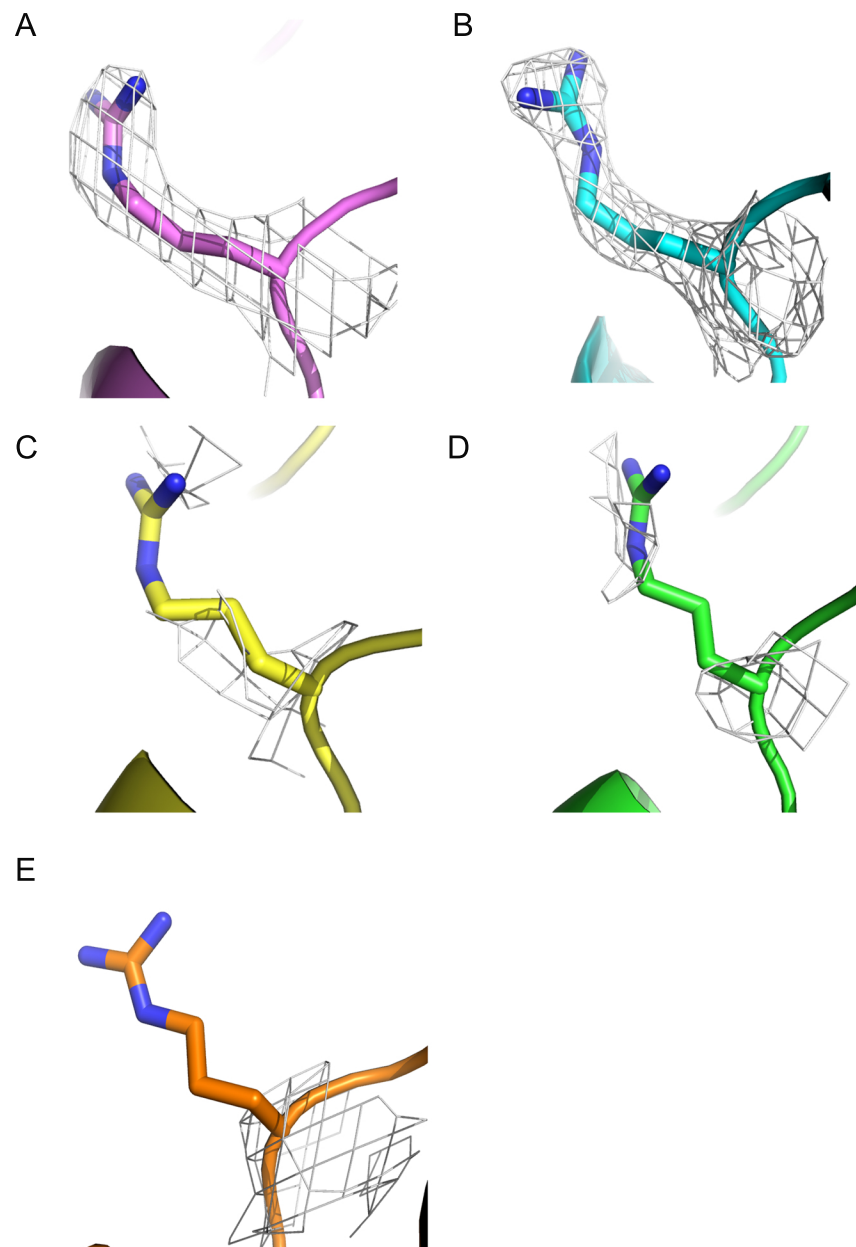
Figure S3. Mobility change revealed for side-chain of the *in trans* Arg-finger residue R359 in $^{\text{ND1}}\text{p97}^{\text{Shrt}}$ and $^{\text{ND1}}\text{p97}^{\text{Lng}}$ Side-chains of the *in trans* Arg-finger residue R359 in stick model from four different ADP-bound structures are overlaid with electron density meshes contoured at 1σ level from their respective $2Fo-Fc$ maps. The

stick models in magenta, cyan, yellow, green and orange are from structures of (A) wild-type ^{ND1}p97^{Shrt}, (B) L198W ^{ND1}p97^{Shrt}, (C) wild-type ^{ND1}p97^{Lng}, (D) R155H ^{ND1}p97^{Lng} and (E) ^{Full}p97 (PDB:3CF2) respectively.



Tang & Xia, Figure.S1





Tang & Xia, Figure S3