Supporting Information

Proline hydroxylation at different sites in hypoxia-inducible factor 1α modulates its interactions with von Hippel–Lindau tumor suppressor protein

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This material contains 1 supplemental table and 3 supplemental figures.

Table S1 The Cα-RMSD between the average structures obtained at the end of the MD simulations run for the eight simulated systems.

Systems	564Hyp-1	564Hyp-2	noHyp-1	noHyp-2
RMSD (nm)	0.17	0.19	0.18	0.20
Systems	567Hyp-1	567Hyp-2	564&567Hyps-1	564&567Hyps-2
RMSD (nm)	0.39	0.19	0.31	0.21

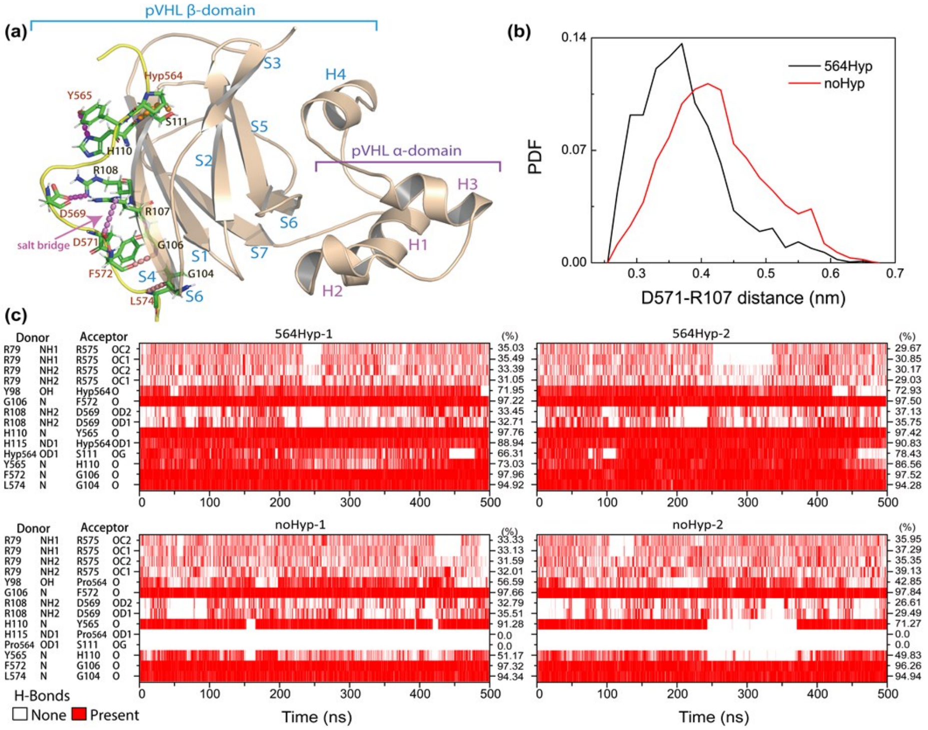

Fig. S1 A representative snapshot of pVHL/HIF-1α complex showing the H-bonds between HIF-1α and pVHL (a). The probability density distribution of the distance between D571 of HIF-1α and R107 of pVHL in 564Hyp (black) and noHyp (red) systems (b). The D571-R107 distance is the minimum distance between the side chain COO^{-} group of D571 and the Nζ atoms of R107. H-bond existence map between pVHL and HIF-1α during each trajectory of MD simulations for 564Hyp and noHyp systems (c). In each plot, H-bond indexes (donor–acceptor pairs) are shown on the left and H-bond incidences are given on the right.

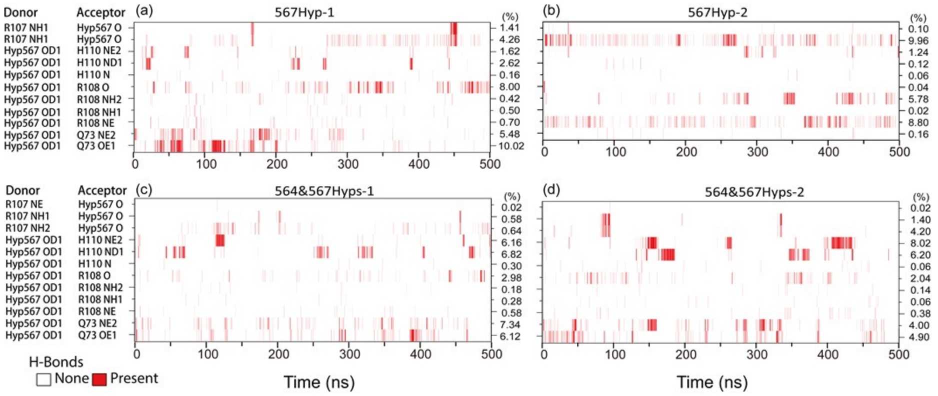

Fig. S2 H-bond existence map involving hydroxylated Pro567 between pVHL and HIF-1α during each MD trajectory for 567Hyp (a, b), and 564&567Hyps (c, d) systems. In each plot, H-bond indexes (donor–acceptor pairs) are shown on the left and H-bond occurrence rates are given on the right.

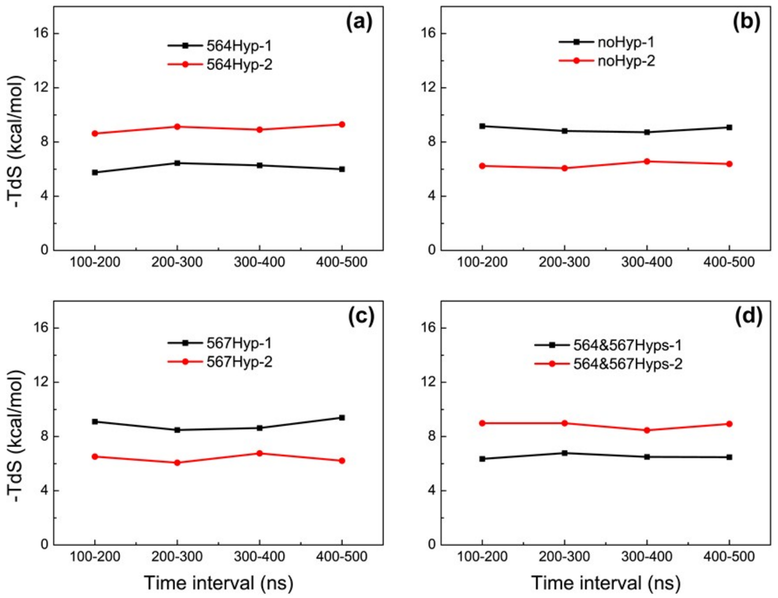

Fig. S3 The convergence of the entropy ($\Delta S_{transl} + \Delta S_{rot}$) by plotting the entropy within four independent time intervals are shown for 564Hyp (a), noHyp (b), 567Hyp (c), and 564&567Hyps (d) systems.