Molecular dynamics study on the inhibition mechanisms of ReACp53 peptide for p53-R175H mutant aggregation

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The authors declare no competing financial interest.

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This material contains eight supplemental figures and one supplemental table.

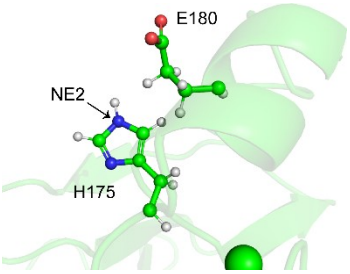

Fig. S1 The protonation state of R175H mutation in p53C.

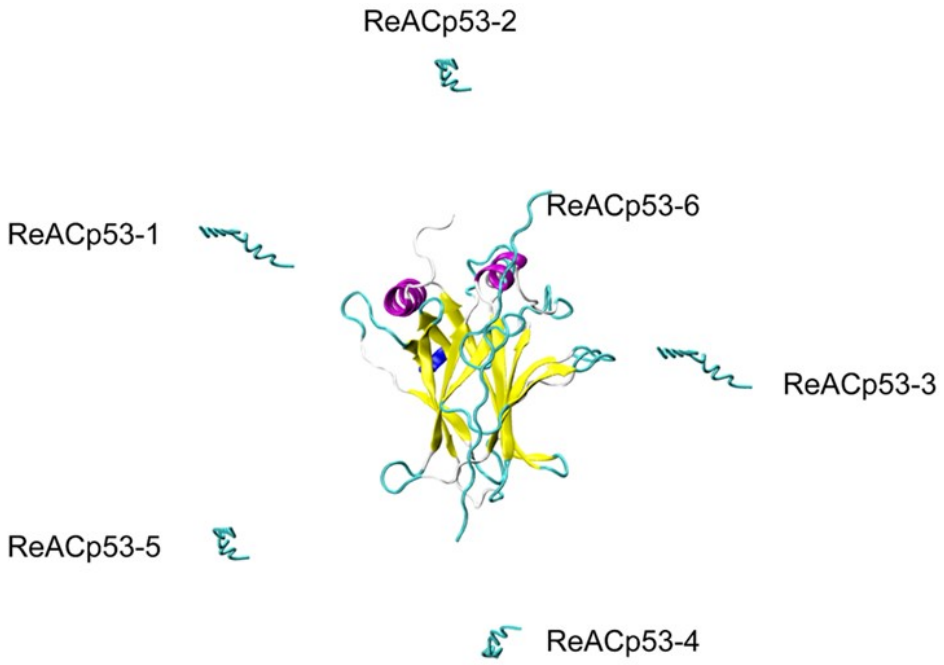

Fig. S2 The six different initial coordinates of R175H mutant with ReACp53 for 6 MDs.

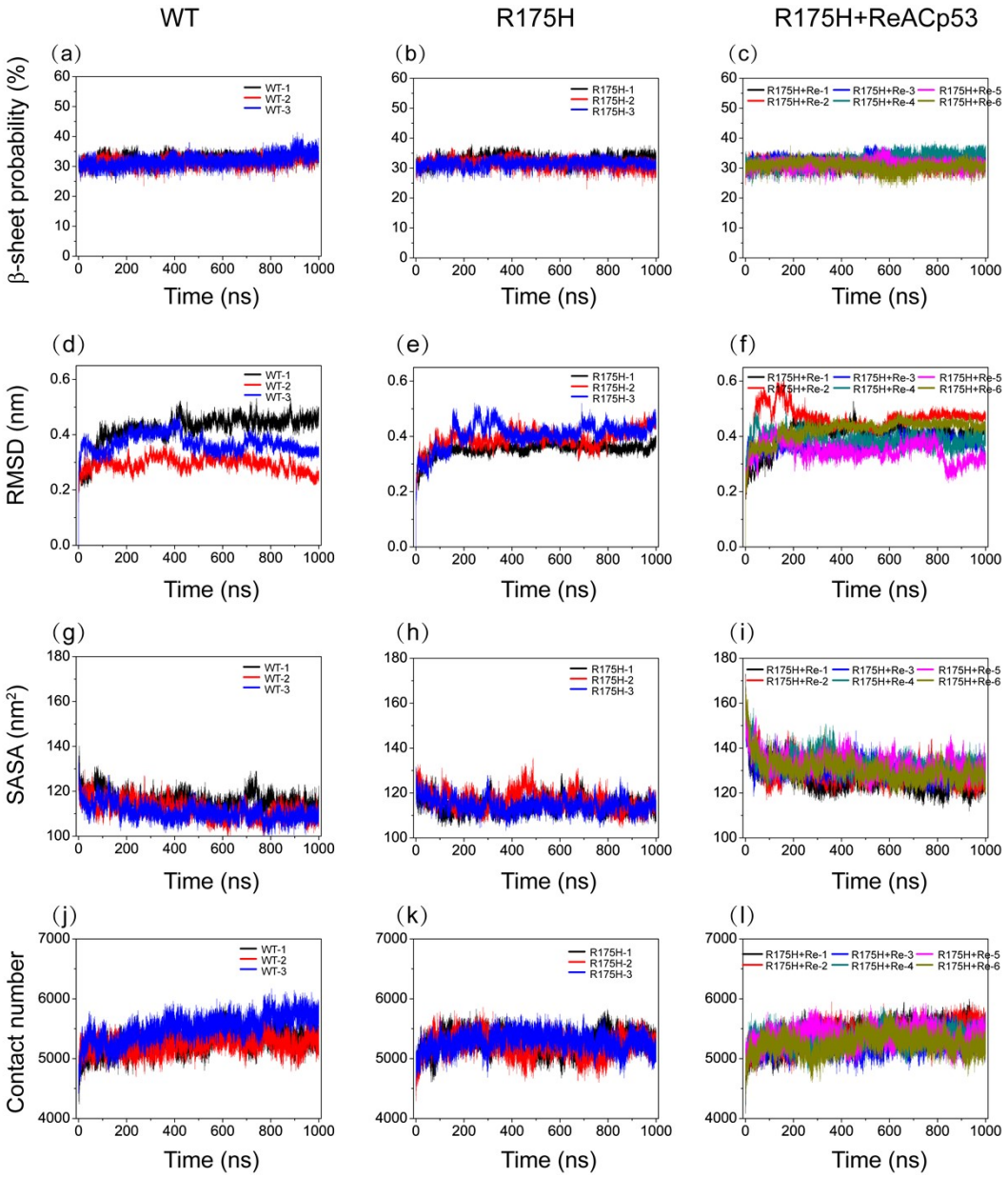

Fig. S3 The convergence analysis of WT, R175H and R175H+ReACp53 systems. Time evolution of the β-sheet probability (a-c), Cα-root-mean-square-deviation (Cα-RMSD) (d-f), the solvent accessible surface area (SASA) (g-i) and contact number of whole p53 protein (j-l).

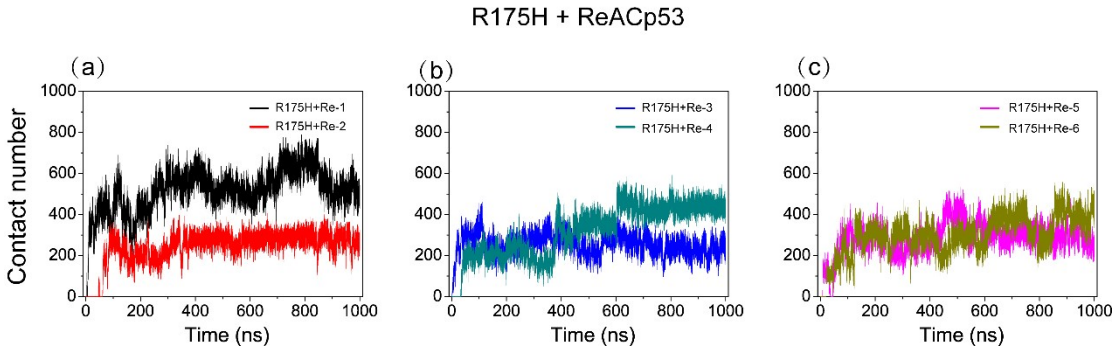

Fig. S4 Time evolution of the contact number between the R175H mutant and ReACp53.

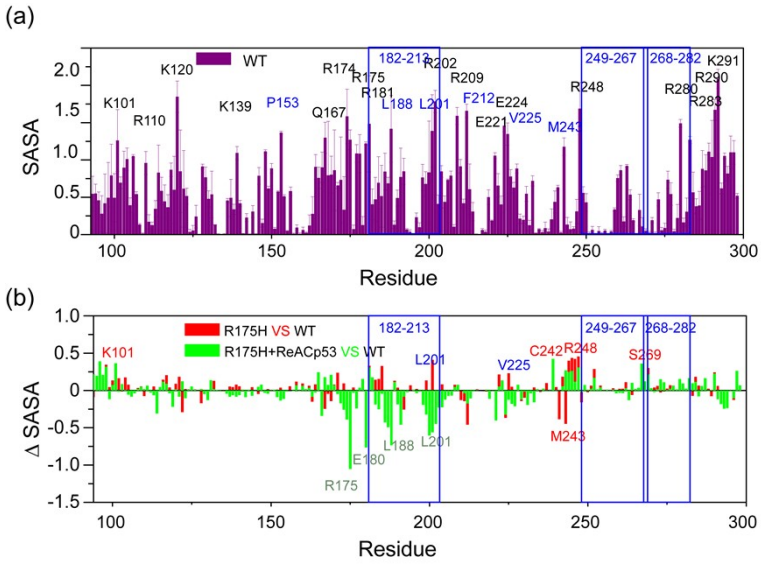

Fig. S5 (a) The solvent accessible surface area (SASA) of each residue in the WT system. (d) The difference value of SASA between R175H mutant (with or without ReACp53) and WT p53C.

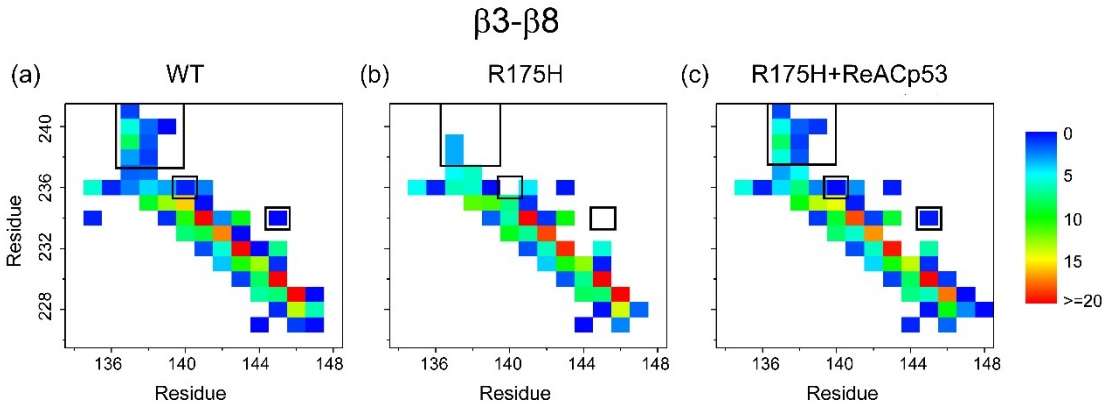

Fig. S6 The maps of contact number between β3 and β8 in the WT (a), R175H (b) and R175H+ReACp53 (c) systems.

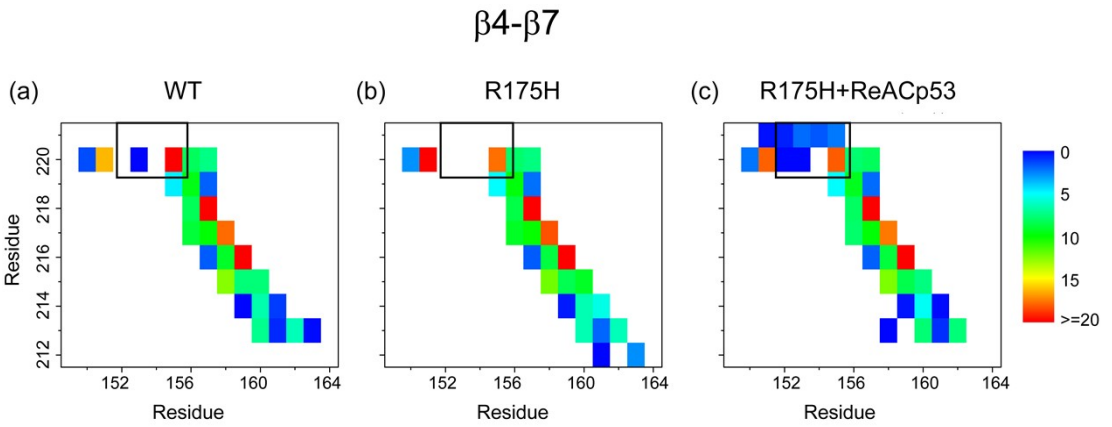

Fig. S7 The maps of contact number between β4 and β7 in the WT (a), R175H (b) and R175H+ReACp53 (c) systems.

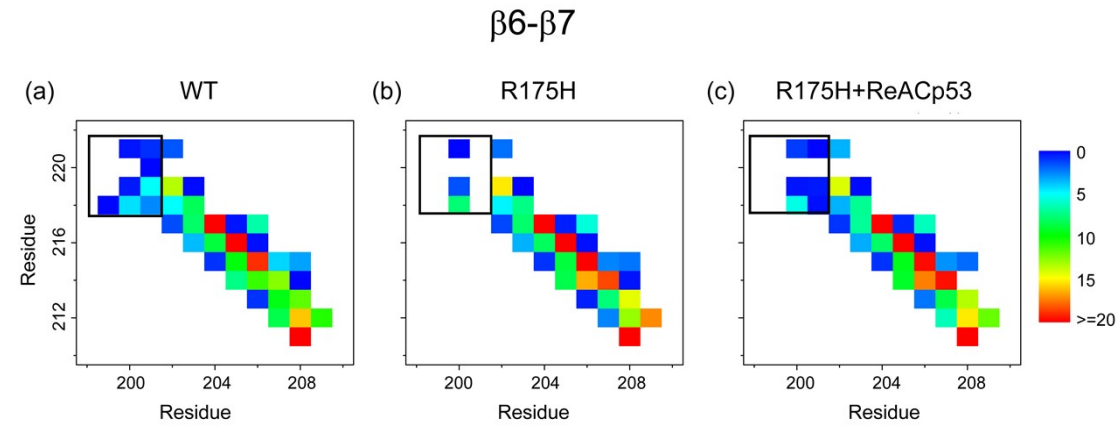

Fig. S8 The maps of contact number between β6 and β7 in the WT (a), R175H (b) and R175H+ReACp53 (c) systems.

Salt bridge	Location	WT (%)	R175H (%)	R175H+ReACp53 (%)
K132-E271	β2′-β10	74.8	66.0	68.9
K132-E285	β2′-H2	94.3	83.1	93.0
R156-E204	β4-β6	13.4	18.4	6.7
R156-D258	β4-β9	64.9	58.5	64.8
R158-D208	β4-β6	12.8	17.6	13.6
R158-D258	β4-β9	99.9	99.9	97.4
K164-E271	β4-β10	80.4	92.8	96.1
R174-E171	L2-L2	36.1	18.0	1.2
R175-E180	L2-L2	44.3	0	0
R175-D184	L2-L2	18.5	0	0
R175-D186	L2-L2	26.4	0	0
R181-E180	L2-L2	17.7	25.9	16.2
R196-D184	L2-L2	43.6	21.6	36.6
R196-D186	L2-L2	23.0	31.3	26.5
R196-E198	β5-β5	44.6	38.5	28.7
R202-E204	L(β5β6)-β6	23.8	7.2	2.3
R202-E221	L(β5β6)-L(β7β8)	15.3	18.6	33.7
R249-E171	L3-L2	60.2	39.1	72.3
R273-D281	β10-H2	50.7	58.3	40.0
R273-E285	β10-H2	48.1	64.7	57.4
R280-D281	H2-H2	33.3	34.5	51.3
R282-E286	H2-H2	99.7	99.5	99.6
R283-E287	H2-H2	65.8	62.6	69.9
R290-D281	H2-H2	33.3	0	16.7
R290-E285	H2-H2	38.9	2.1	39.4
R290-E287	H2-H2	27.1	2.5	4.8

Table. S1 The probabilities of salt bridge pairs in p53C for WT, R175H and R175H+ReACp53.