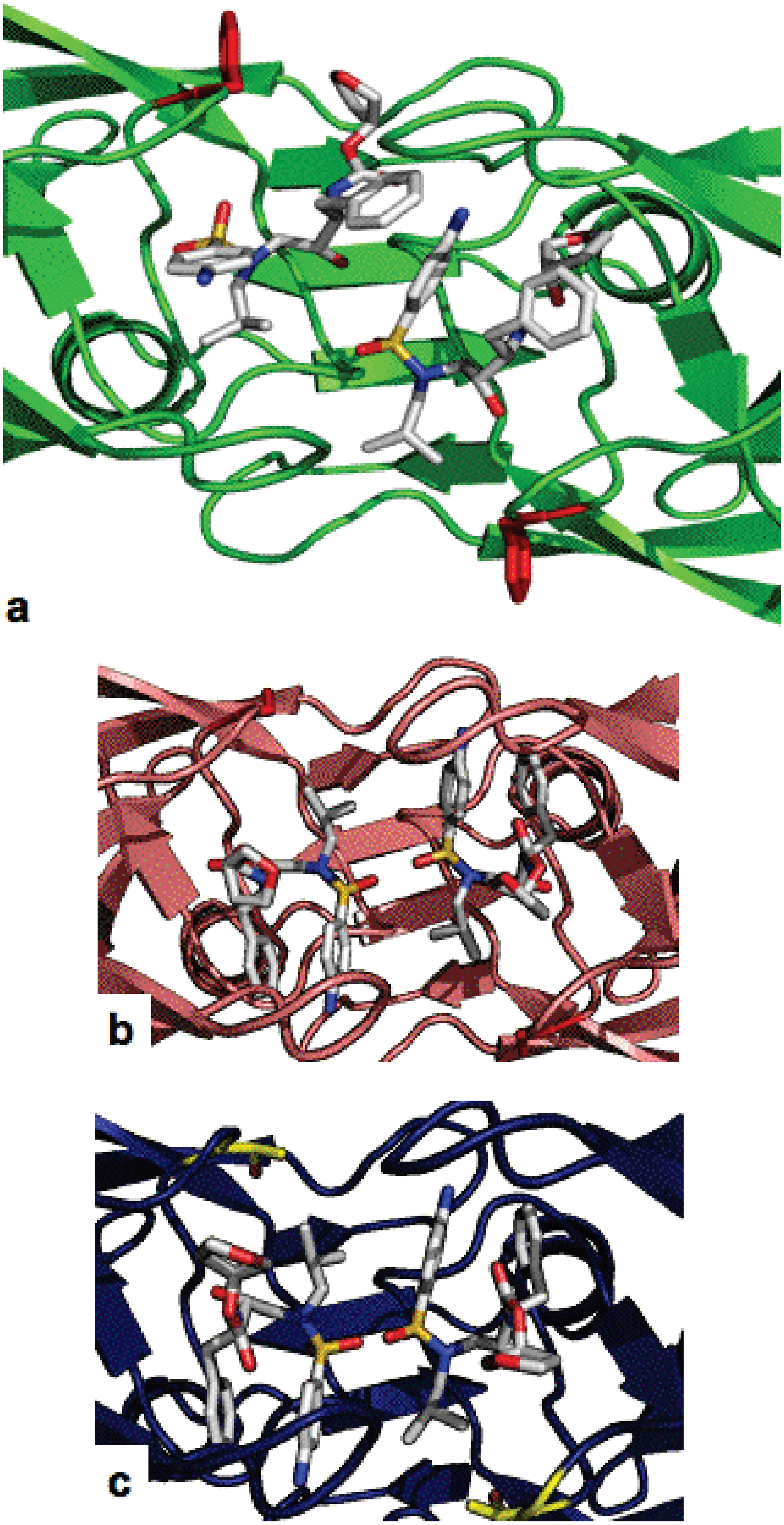
Supplementary Material

Supplementary Table 1. List of currently available HIV-1 protease apo-protein structures.

PDB entry	Resolution (Å)	Space group	No. of mutations	Remarks
2HVP	3.0	$P4_{1}2_{1}2$	0	Wild type
3HVP	2.8	$P4_{1}2_{1}2$	6	2X mutant
3PHV	2.7	$P4_{1}2_{1}2$	1	Wild type
1HHP	2.7	$P4_{1}2_{1}2$	1	Wild type
1GL6	1.9	$P6_{1}$	3	Wild type
1LV1	2.1	$P6_{1}$	3	Wild type
1Q9P	N/A	NMR	5	Wild type
1RPI	1.86	$P4_{1}$	10	9X mutant
1TW7	1.3	$P4_{1}$	11	10X mutant
2G69	1.35	$P4_{1}2_{1}2$	6	1X mutant
2HB2	2.3	$P4_{1}2_{1}2$	7	6X mutant
2HB4	2.15	$P4_{1}2_{1}2$	1	Wild type

N/A - Not available


a
b
c

Supplementary Figure 1. Docking studies with amprenavir. Shown here are the docked models of MDR769 HIV-1 protease variants. *(a)* A82F mutant shown in green with Phe82 highlighted as red stick model. *(b)* A82S mutant shown in light pink with Ser82 highlighted as red stick model. *(c)* A82T mutant shown in dark blue with Thr82 highlighted as yellow stick model. Each model shows two molecules of amprenavir (white color stick representation) docked into the expanded active site cavity without steric clashes suggesting the conserved trend of expanded active site cavity among the variants.