Structures of Darunavir-Resistant HIV-1 Protease Mutant Reveal Atypical Binding of Darunavir to Wide Open Flaps

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Table S1. Crystallographic Data Collection and Refinement Statistics

Complex name	$PR_{P51\text{-}D25N}$/DRV	$PR_{P51\text{-}D25N}$
Wavelength (Å)	1.0	1.0
Space group	$P4_12_12$	$P4_1$
Unit cell dimensions (Å) a = b c α = β = γ	 46.80 100.63 90°	 46.69 101.62 90°
Unique reflections	13867	34414
Redundancy[§]	8.3 (4.6)	8.0 (3.4)
R_{merge} (%) overall[§]	8.1% (42.2%)	6.7% (27.7%)
<I/sigma> overall[§]	18.5 (3.3)	23.2 (4.6)
Completeness (%) overall[§]	99.4% (98.3%)	99.4% (95.5%)
Refinement resolution range	22.16-1.66	23.64-1.50
R_{work}	18.9%	15.9%
R_{free}	22.6%	19.7%
No. of water molecules atoms (total occupancies)[¶]	48 (45.5)	144 (119.5)
RMSD from ideality		
Bonds (Å)	0.021	0.023
Angle distance (degrees)	2.326	2.070
Average B-factors ($Å^2$)		
Main chain atoms	26.33	23.17
Side chain atoms	31.10	27.88
Ligand	33.10	-
Solvent	35.35	32.43

[§]Values in parentheses are given for the highest resolution shell
[¶]Values in parentheses are given for total occupancies

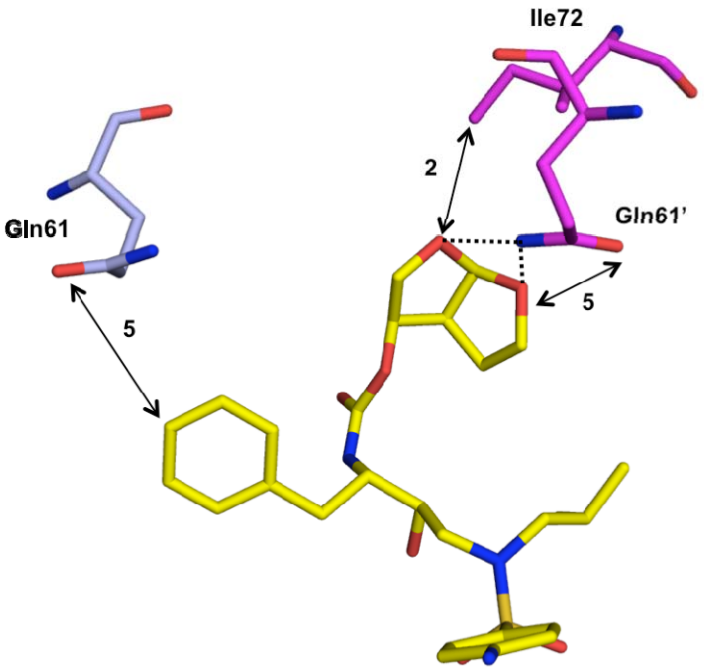

Figure S1. DRV interactions with symmetry-related monomer of $PR_{P51\text{-}D25N}$. The dotted lines show the hydrogen bond interactions and the double-sided arrows represent the van der Waals contacts. The numbers of van der Waals contacts are indicated.

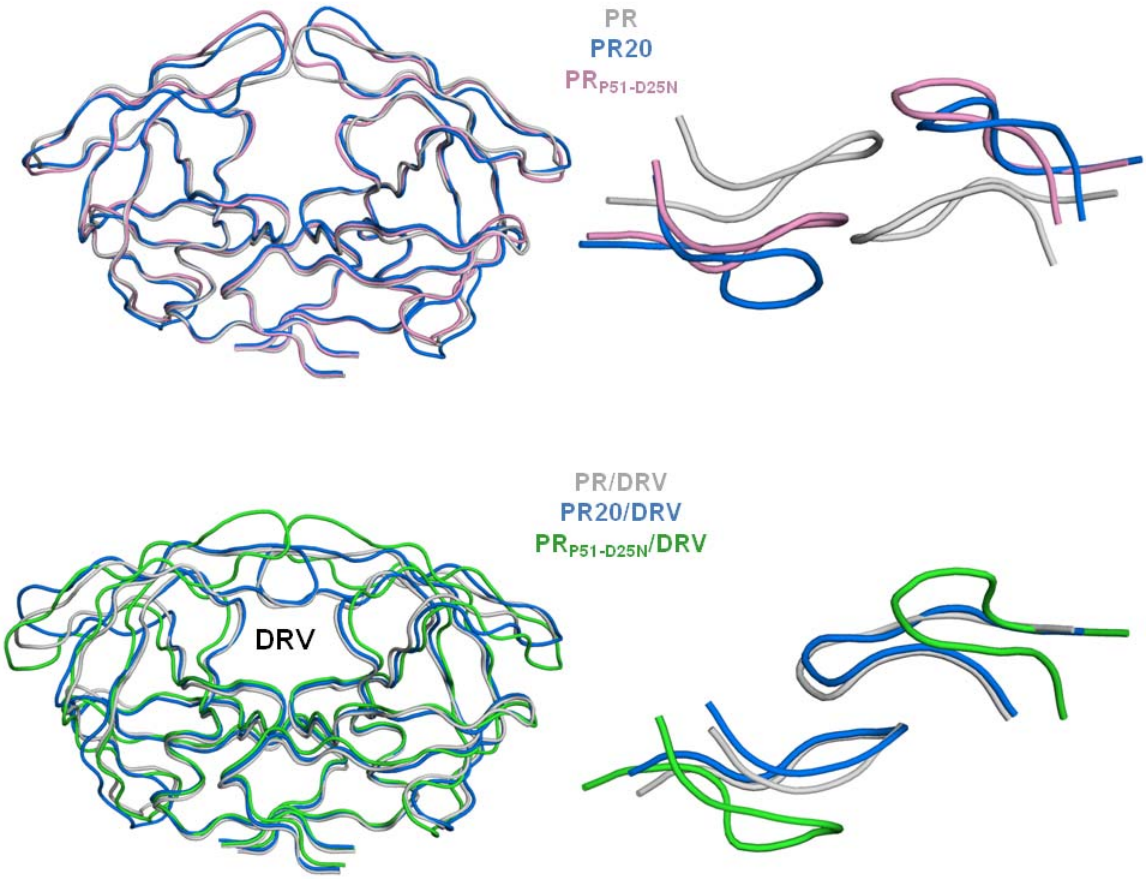

Figure S2. Comparison of $PR_{P51-D25N}$, PR20 and wild-type PR structures. (A) Superposition of ligand-free PR (PDB ID: 1HHP) (grey), PR20 (PDB ID: 3UF3) (blue) and $PR_{P51-D25N}$ (pink) in ribbon representation with perpendicular view of flap residues 46-54. (B) Superposition of PR/DRV (PDB ID: 2IEN) (grey), PR20/DRV (PDB ID: 3UCB) (blue) and $PR_{P51-D25N}$/DRV (green) in ribbon representation and perpendicular view of residues 46-54. DRV is omitted for clarity.