

Supporting Information Available

Figure S1 for the RMSD and some key internuclear distances *versus* the simulation time for wild-type HIV-1 protease binding with inhibitors; Figure S2 for comparison between the X-ray structures of the WT and mutated HIV-1 protease; Figure S3 for the RMSD and some key internuclear distances *versus* the simulation time for SQV binding with the I54M mutant, APV binding with the V82F mutant, and IDV binding with the R8Q mutant; Tables S1 to S9 for the detailed energetic results in comparison with the corresponding experimental data. Tables S10 for the comparison between the X-ray structures of the WT and mutated HIV-1 protease in the RMSD of the backbone and ligand atoms. This material is available free of charge *via* the Internet at <http://pubs.acs.org>.

References

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