Supporting Information For

Understanding the effect of drug-resistant mutations of the HIV-1 intasome on the raltegravir action through molecular modeling study

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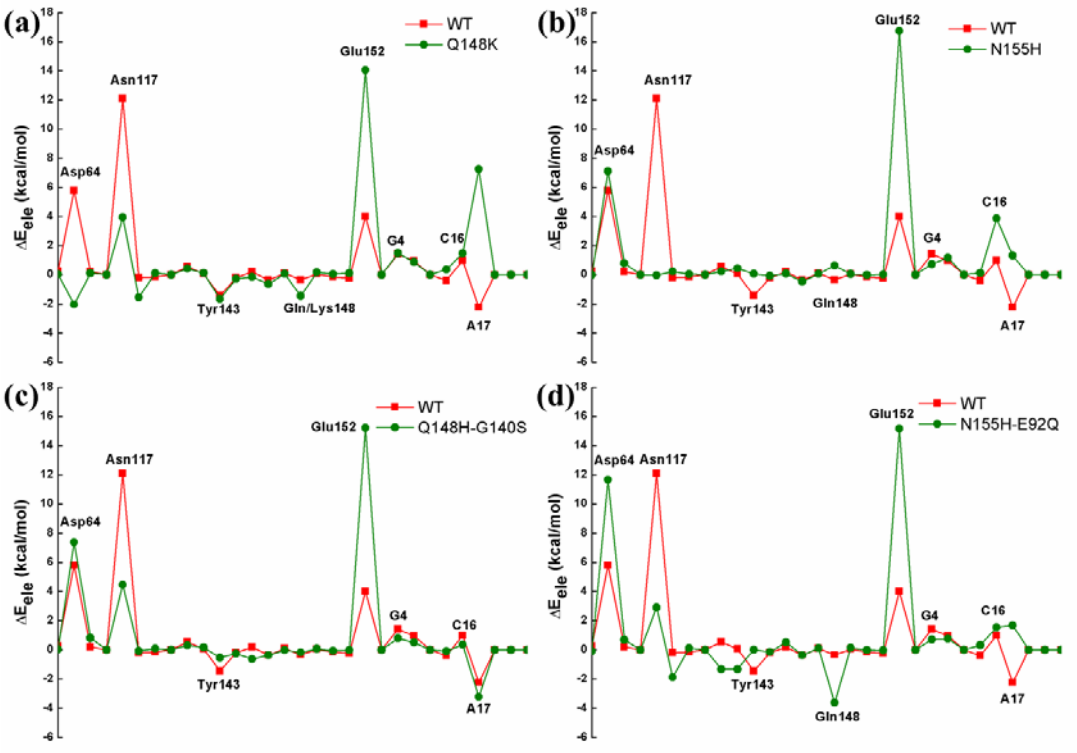

Figure S1. The nonbonded intermolecular electrostatic (ΔE_{ele}) interactions between intasome (residue in the active site) with raltegravir. Red lines represent the wild-type model, and green lines represent the mutant model.

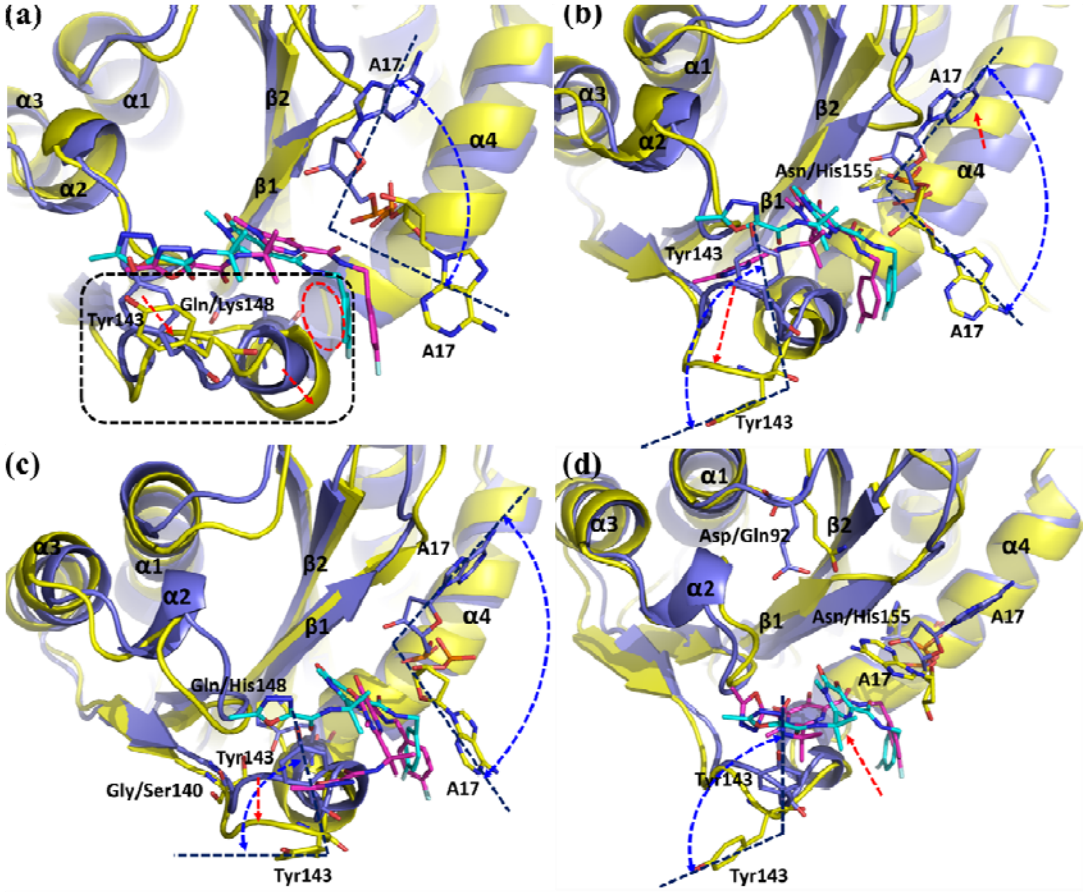

Figure S2. Superimposition of the MD-simulated structures of the wild-type HIV-1 intasome-raltegravir complex and (a) Q148K, (b) N155H, (c) Q148H-G140S and (d) N155H-E92Q mutant. Cartons of the wide-type (purple) and mutant (yellow) in the MD-simulated structures are shown. Raltegravir is shown as a stick representation in the wild-type (cyan) and mutant (pink) systems.

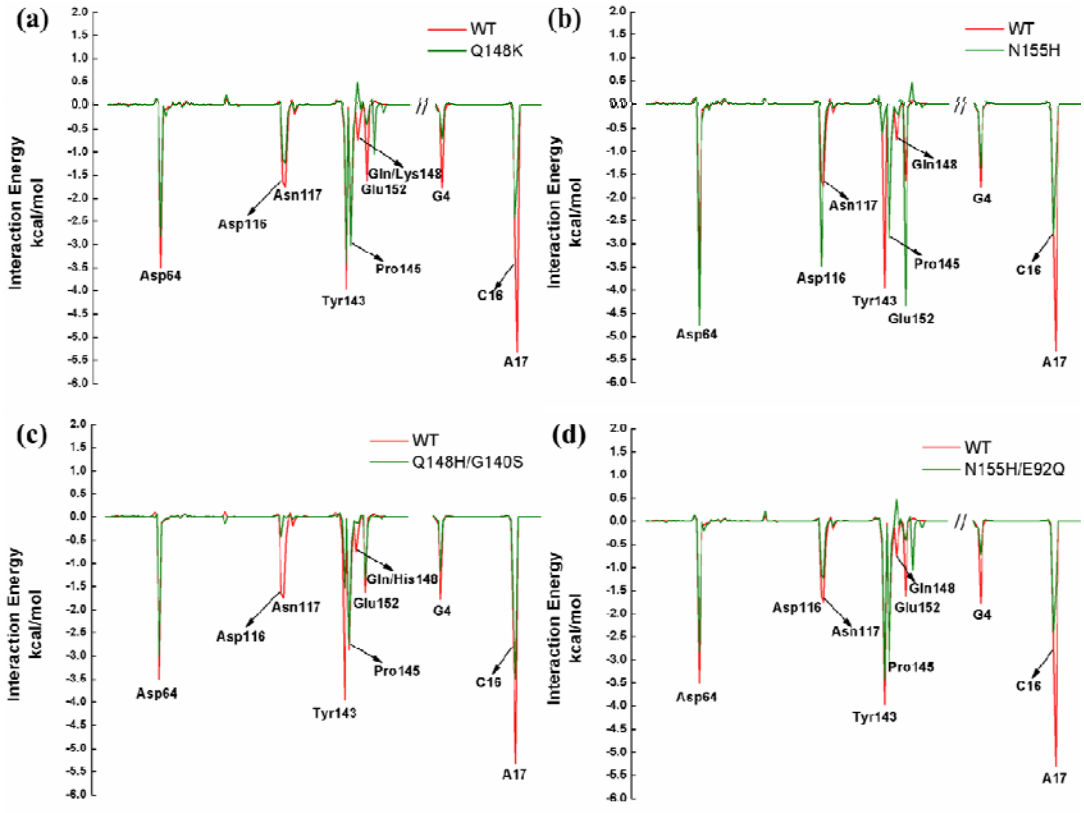

Figure S3. Intermolecular ligand receptor (per-residue) interaction spectrum of the wild-type and mutant intasome-raltegravir complexes according to the MM-GBSA method. Red lines represent the wild-type model, and green lines represent the mutant model.

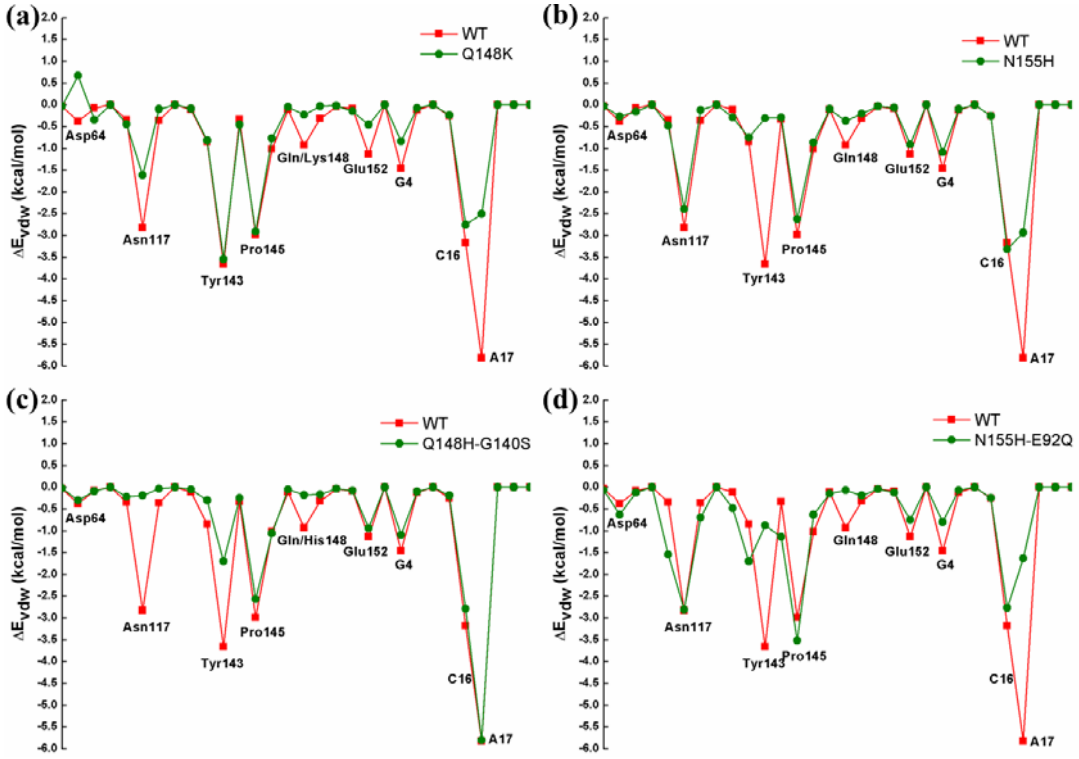

Figure S4. The nonbonded intermolecular van der Waals (ΔE_{vdw}) interactions between intasome (residue in the active site) with raltegravir. Red lines represent the wild-type model, and green lines represent the mutant model.

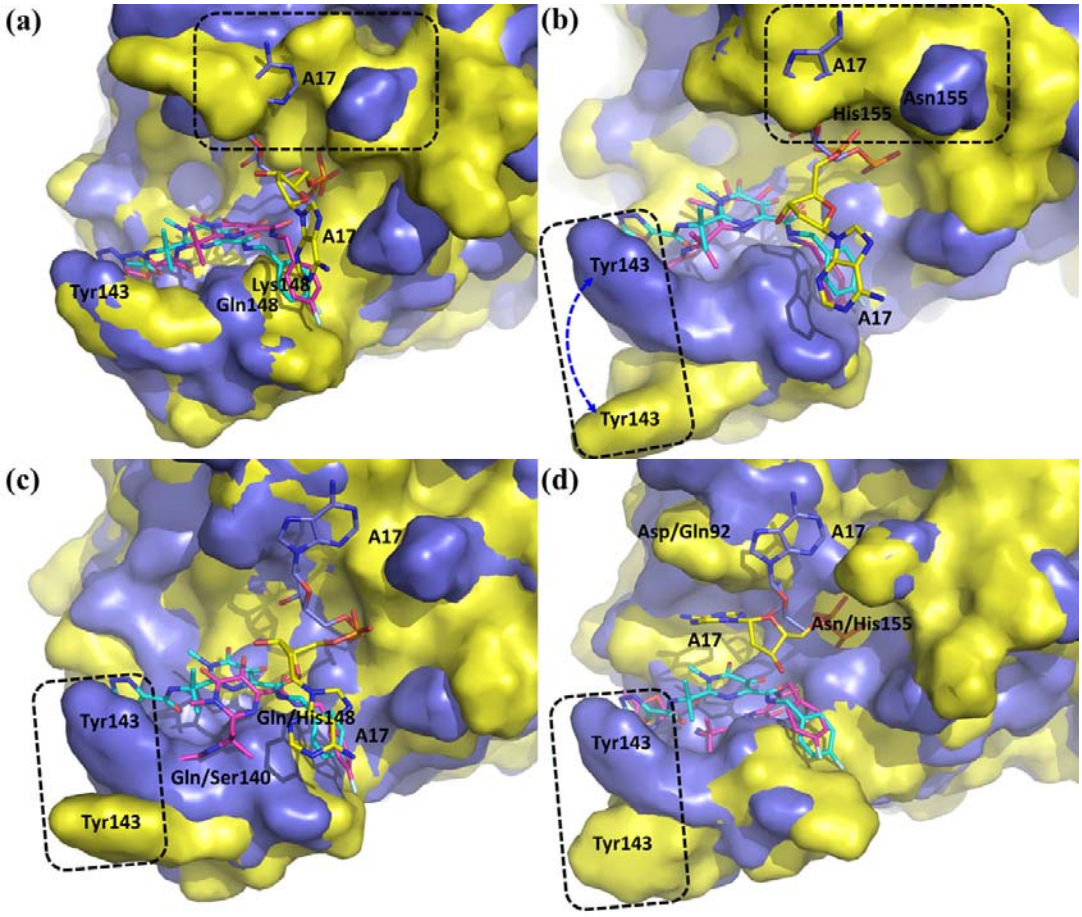

Figure S5. The molecular surface superimpositions of the wild-type (purple) and (a) Q148K, (b) N155H, (c) Q148H-G140S and (d) N155H-E92Q mutant (yellow) HIV-1 integrase active site. Purple (wild-type) and yellow (mutant) stick representations are shown for the viral DNA 3' adenosine. Raltegravir is also shown as a stick representation in the wild-type (cyan) and mutant (pink) systems.