

## Supplementary material:

**Table 1:** HBVrt amino acid residues involved in the H-bond interaction with adefovir

Protein	Interacting Residues	H-Donors	H-Acceptors	Binding Energy (kcal/mol)	VdW+Electrostatic energy+hbond (kcal/mol)
HBVrt wild type (rtI233)	Asp83 (2.904 Å)	UNK`1/O30	Asp83/OD2	-5.97	-9.35
	Asp205 (2.792 Å)	MG`601/Mg	Asp205/OD2		
	Mg (2.053 Å)	MG`600/Mg	UNK1/O6		
	Arg41 (2.797 Å)	Arg41/2HH1	UNK1/O6		
	Arg41 (2.888 Å)	UNK`1/O11	Asn33/OD1		
HBVrt mutant (rtI233V)	Asn33 (2.876 Å)	Arg41/NH2	UNK1/O11	-5.19	-9.14
	Lys32 (2.787 Å)	Lys32/NZ	UNK1/O6		
	Mg (2.259 Å)	MG`600/Mg	UNK1/O7		
	Arg41 (2.580 Å)	Arg41/2HH2	UNK1/O7		
	Arg41 (2.888 Å)	Arg41/NH1	UNK1/O7		