The structural basis of Mos1 transposase inhibition by the anti-retroviral drug Raltegravir.

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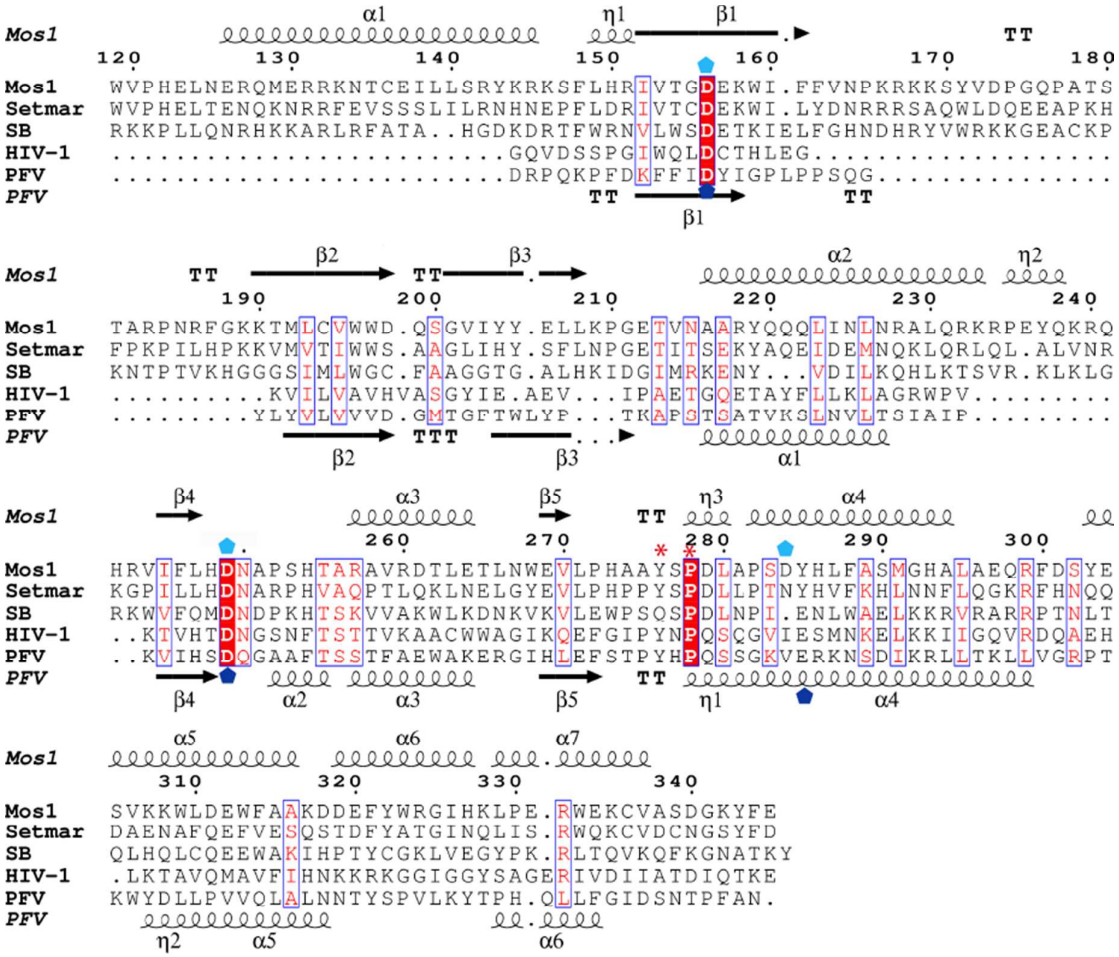
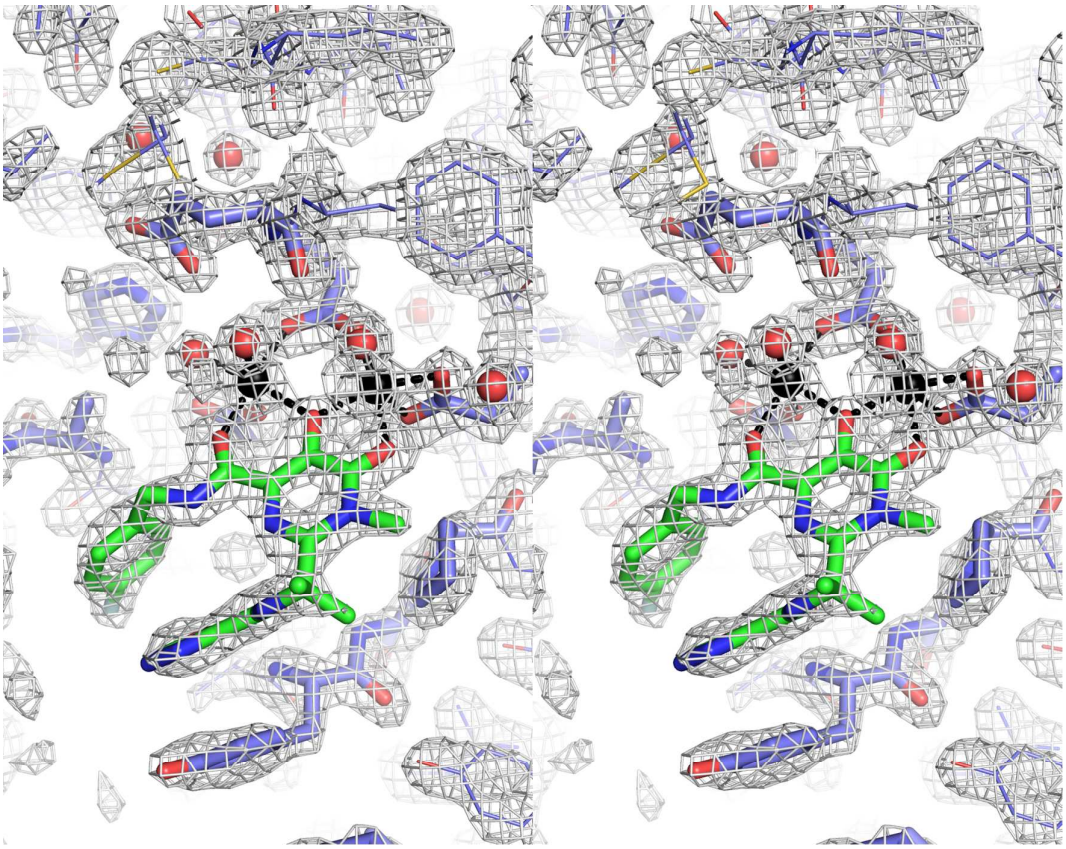
Supplementary Figures

Supplementary Figure 1. Structure based sequence alignments of the catalytic core domains of Mos1, Setmar, Sleeping Beauty (SB), HIV-1 integrase and PFV integrase. Secondary structure elements of Mos1 (from PDBID: 3HOT) and PFV catalytic domains (from 3S3M) are shown above and below the alignments, respectively. Conserved residues are shown in white on a red background and similar residues are highlighted in red. TT represents a β-turn. The residues of the DD-34-D/N and DD-35-E motifs are highlighted by light and dark blue pentagons respectively. The conserved Tyr and Pro residues preceding the third active site residue are marked by red asterisks.



Supplementary Figure 1

Supplementary Figure 2. Stereo view of the Mos1-Raltegravir co-crystal structure with Mg^{2+} in the active site (PDBID: 4MDB) showing the final $2f_o$-f_c electron density map contoured at 1.5σ.



Supplementary Figure 3. Stereo view of the Mos1-Raltegravir co-crystal structure with Mn^{2+} in the active site (PDBID: 4MDA) showing the final $2f_o$-f_c electron density map contoured at 1.5σ.