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Supplemental Material to:

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Crystal structure of HIV-1 Tat complexed with human P-TEFb and AFF4

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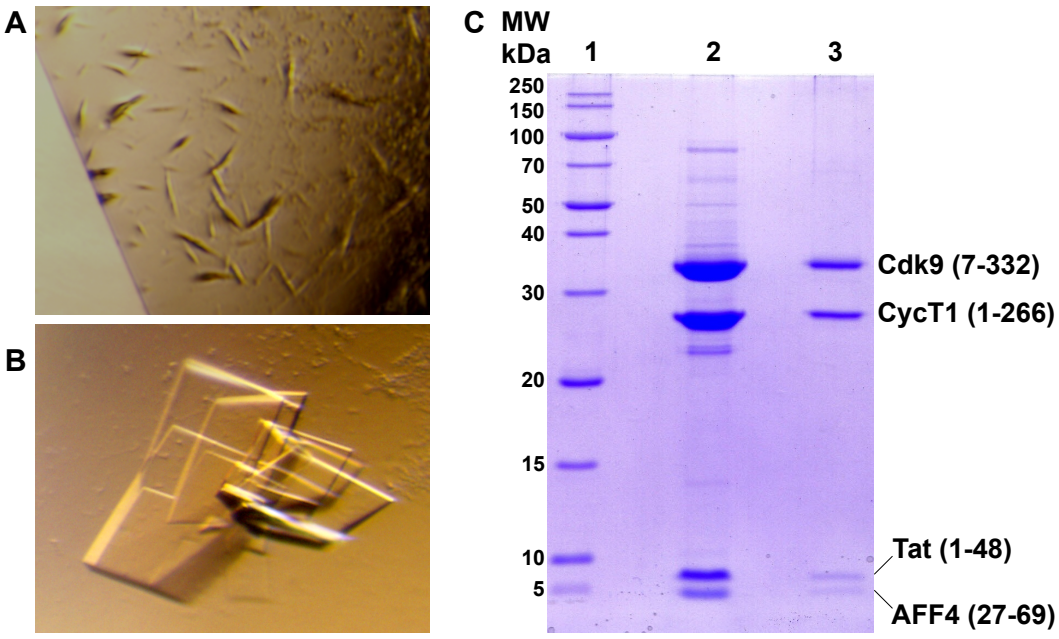

Figure S1. Crystals of Tat•AFF4•P-TEFb complex. Photomicrographs of (**A**) the best crystals after initial screens and (**B**) plate crystals grown in presence of YCl_3. (**C**) Composition of dissolved crystals verified by SDS-PAGE. Lane 1 is a molecular weight marker, lane 2 is a protein sample used for crystallization and lane 3 is a solution of dissolved crystals.

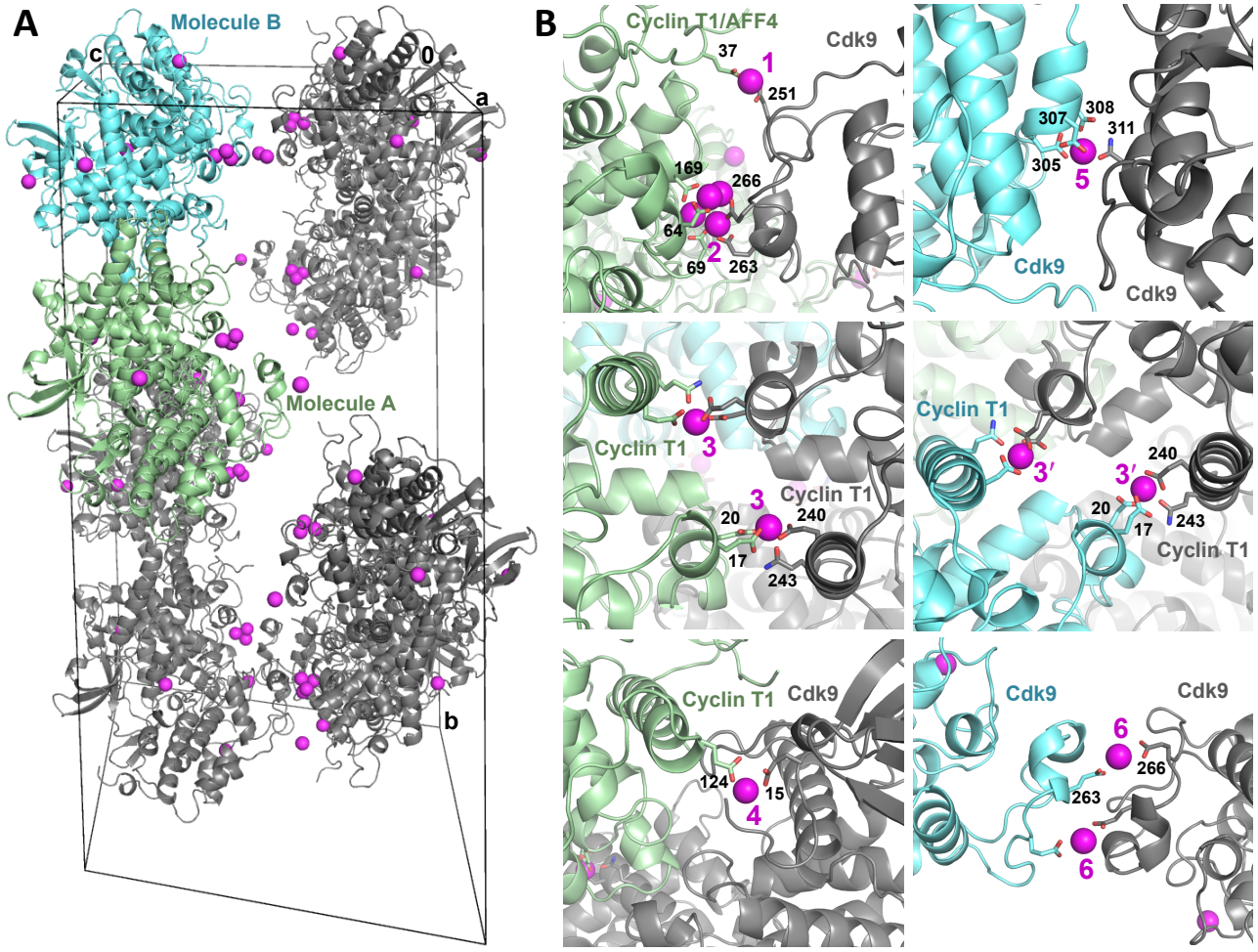

Figure S2. Participation of yttrium ions in Tat•AFF4•P-TEFb crystal packing. (**A**) Location of Tat•AFF4•P-TEFb molecules in the unit cell. Two independent molecules A and B in an asymmetric unit are colored in pale green and cyan, respectively. Symmetry-related molecules are in grey. Proteins are displayed as cartoons and yttrium ions are displayed as magenta spheres. (**B**) Close view of yttrium ions mediating interactions of Tat•AFF4•P-TEFb molecules A (pale green) and B (cyan) with neighboring molecules (gray) at sites 1-4 for molecule A and 5, 3' and 6 for molecule B. Only site 3 for molecule A has an equivalent site 3' for molecule B. The amino-acid residues participating in yttrium coordination and contributing subunits of Tat•AFF4•P-TEFb are labeled.

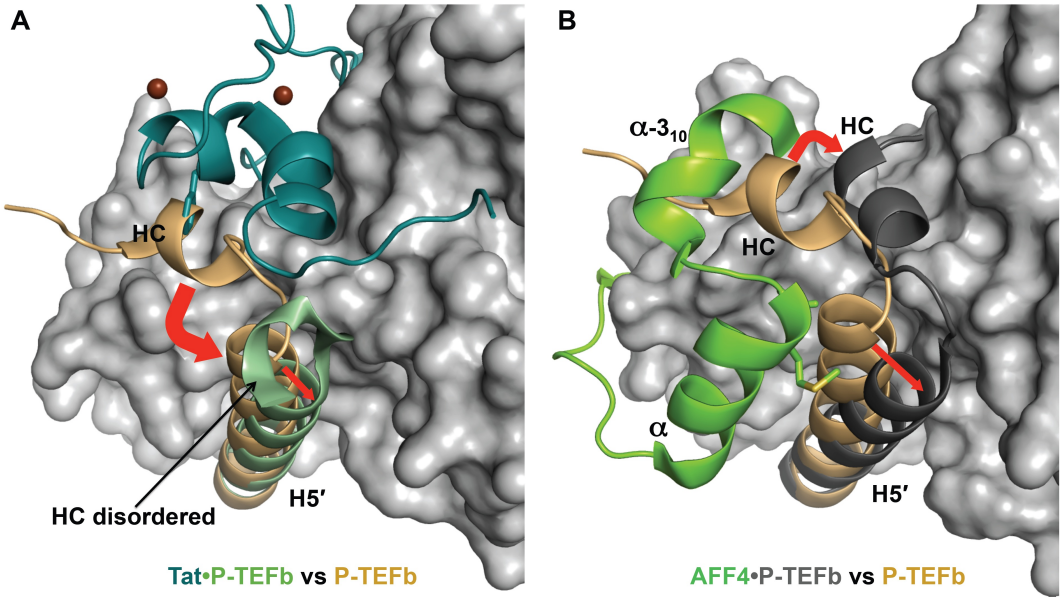

Figure S3. Comparison of Tat•P-TEFb and AFF4•P-TEFb structures with P-TEFb. Comparison of (**A**) Tat•P-TEFb with P-TEFb and (**B**) AFF4•P-TEFb with P-TEFb. Red arrows indicate the directions of P-TEFb structural elements shifts that occur upon binding of Tat or AFF4.

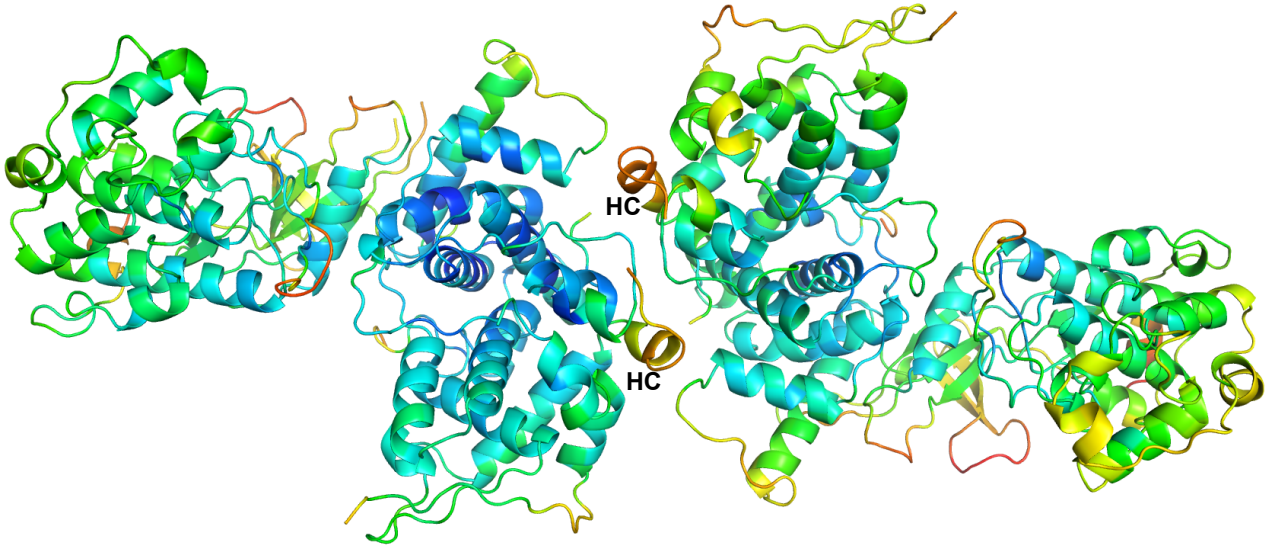

Figure S4. Distribution of B-factors in structure of Tat•AFF4•P-TEFb. Both independent Tat•AFF4•P-TEFb molecules are shown. The spectrum is changing from blue (the lowest B-factor value of 8 Å^2) to green, yellow and red (the highest B-factor value of 140 Å^2).