PROTEIN STRUCTURE AND FOLDING:

Supplementary materials for

Structural basis for acetylated histone H4 recognition by the human BRD2 bromodomain

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SUPPLEMENTARY FIGURE LEGENDS

SUPPLEMENTARY FIGURE 1. Crystal packing of the BRD2-BD1 bromodomain complex with the acetylated histone H4 peptide P1. Crystal packing of the BD1 complex in the unit cell is shown. The non-crystallographic symmetry (NCS) molecules A and B form a homodimer, while the NCS molecule C forms a homodimer with the symmetry related molecule C'. The NCS molecules A, B and C of BD1 are colored in blue, red and hot pink, respectively. The corresponding symmetry related molecules are colored in green, cyan and light pink, respectively. The peptide chains in the NCS are shown as sticks model for clarity. The unit cell is shown with green lines.

SUPPLEMENTARY FIGURE 2. The BRD2-BD1 interaction with the acetylated histone H4 peptide P1. *A*, Stereo-view of the refined peptide bound to molecule A of BD1. *B*, Stereo-view of the refined peptide bound to molecule B of BD1. The final electron density 2Fo-Fc maps were contoured at 1.0 σ.

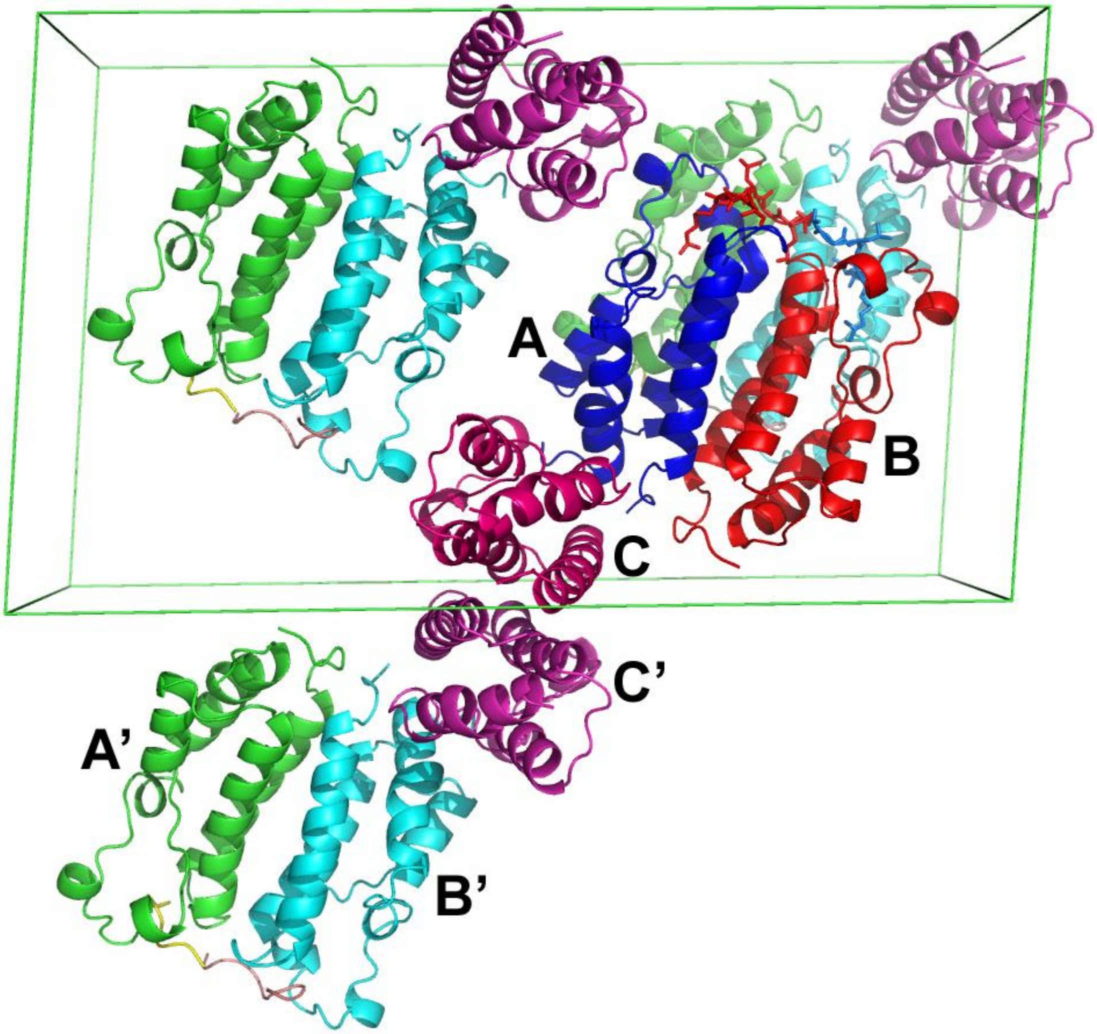
SUPPLEMENTARY FIGURE 3. The BRD2-BD1 interaction with the acetylated histone H4 peptide P2. Stereo-view of the refined peptide (6 – 15) bound to molecule B of BD1. The final electron density 2Fo-Fc map is contoured at 0.9 σ.

SUPPLEMENTARY FIGURE 4. The BRD2-BD1 interaction with the acetylated histone H4 peptide P3. *A*, The refined weakly-bound H4K12ac with molecule A of the BD1 dimer. The electron density for the other residues of the peptide is completely absent. *B*, The refined H4K12ac bound to molecule B of the BD1 dimer. The electron density for the rest of the peptide is also completely absent. The final electron density 2Fo-Fc maps are contoured at 0.9 σ.

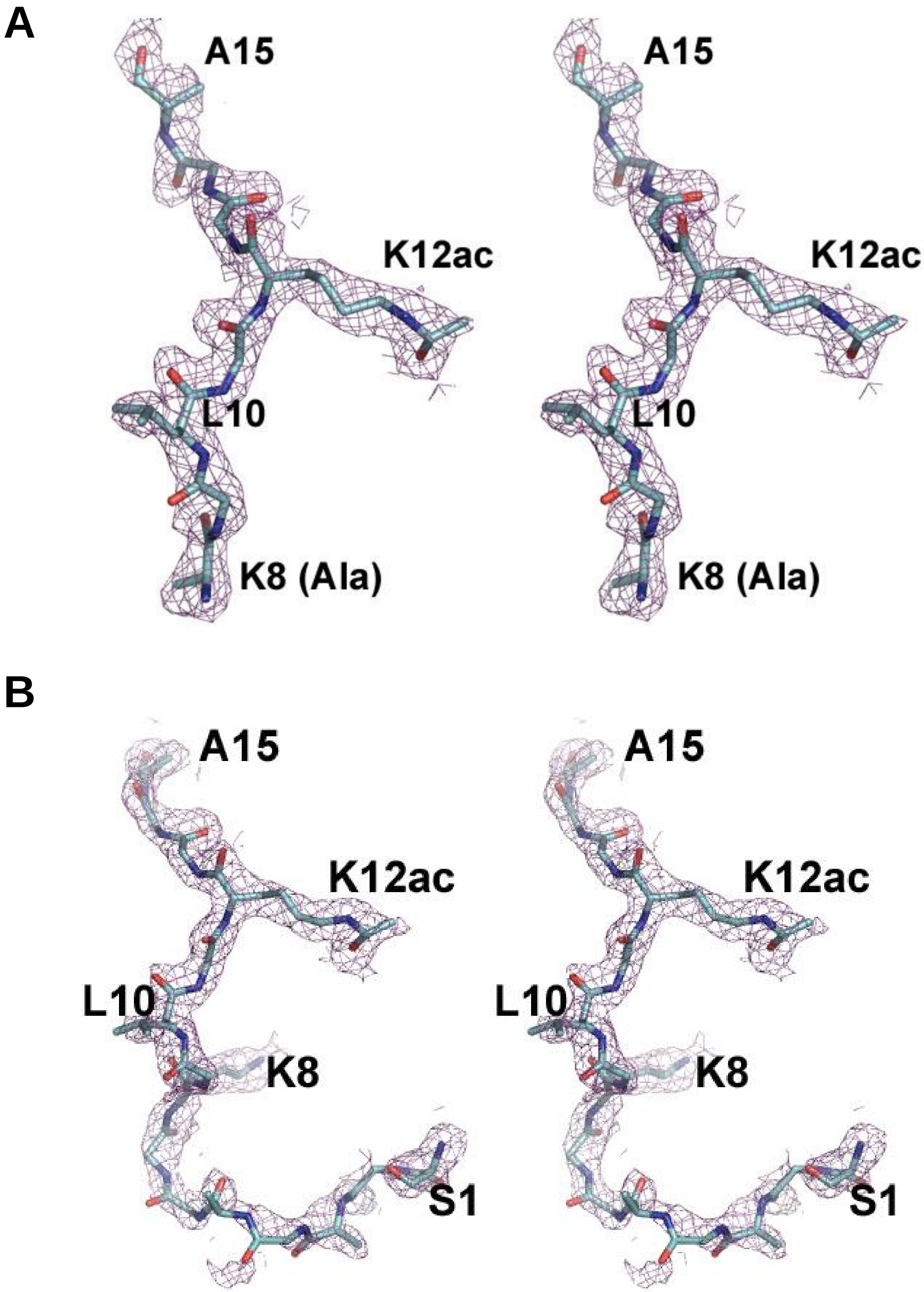
SUPPLEMENTARY FIGURE 5. Comparison of the structures of the BRD2-BD1 and BRDT-BD1 complexes. Superposition of BRD2-BD1 of the BRD2-BD1 complex on to BRDT-BD1 of the BRDT-BD1 complex. The color code: red, BRD2-BD1 complex; and grey, BRDT-BD1 complex. The peptides are shown as sticks model, and the acetylated lysine residues are labeled corresponding to their respective chain colors.

SUPPLEMENTARY FIGURE 6. Comparison of BRD2-BD1 and the TAF1 double bromodomains. Stereo-view of superposition of one of the BRD2-BD1 homodimer with the first bromodomain of TAF1 is shown with the color code: blue and red, BD1 homodimer; green and cyan for carbon atoms, H4 peptides; and slate, the first bromodomain of TAF1.

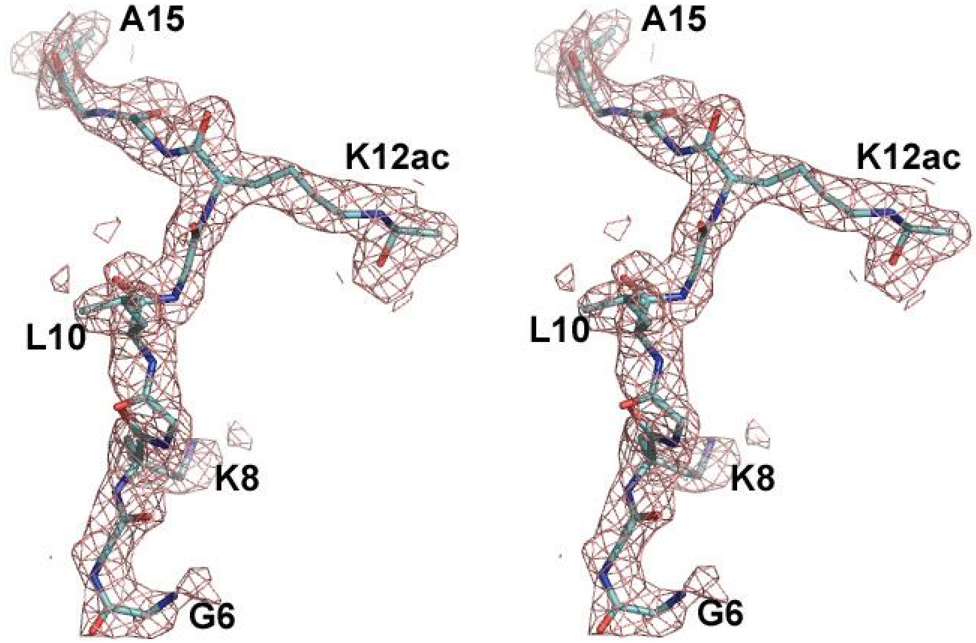
Supplementary Figure 1



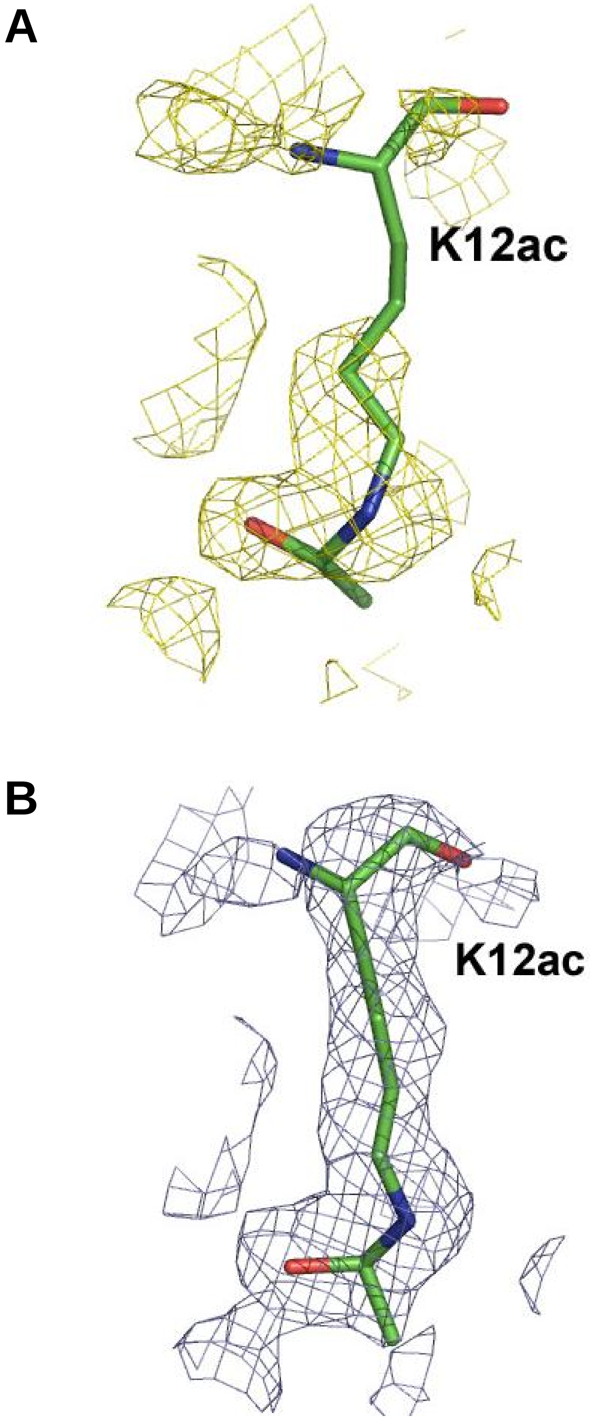
Supplementary Figure 2



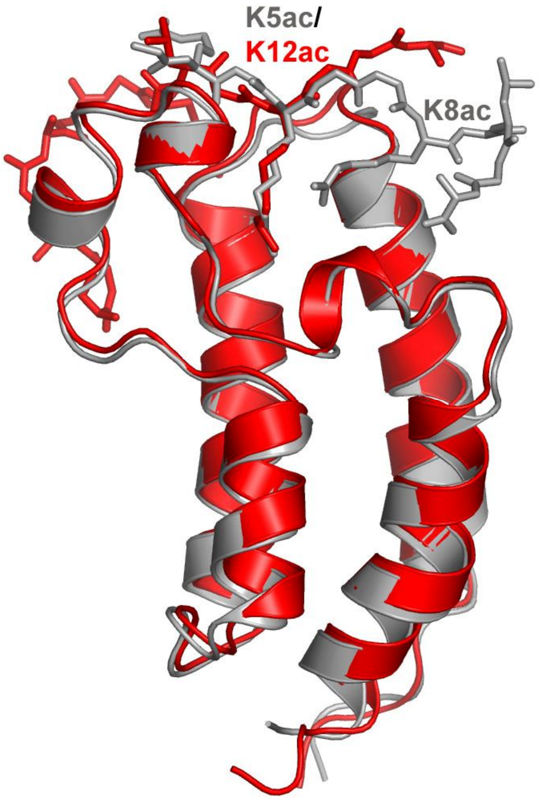
Supplementary Figure 3



Supplementary Figure 4



Supplementary Figure 5



Supplementary Figure 6