

Supplemental Information

Figure 1: Plot of R_{free} (left Y axis, black), total X-ray potential (second left Y axis, green), X-ray free likelihood (right Y axis, red) and total chemical potential (second right Y axis, blue) versus w_A (logarithmic scale) for six representative structures ranging from 2.2 to 4.0 Å (PDB IDs and resolutions are given above each respective plot).

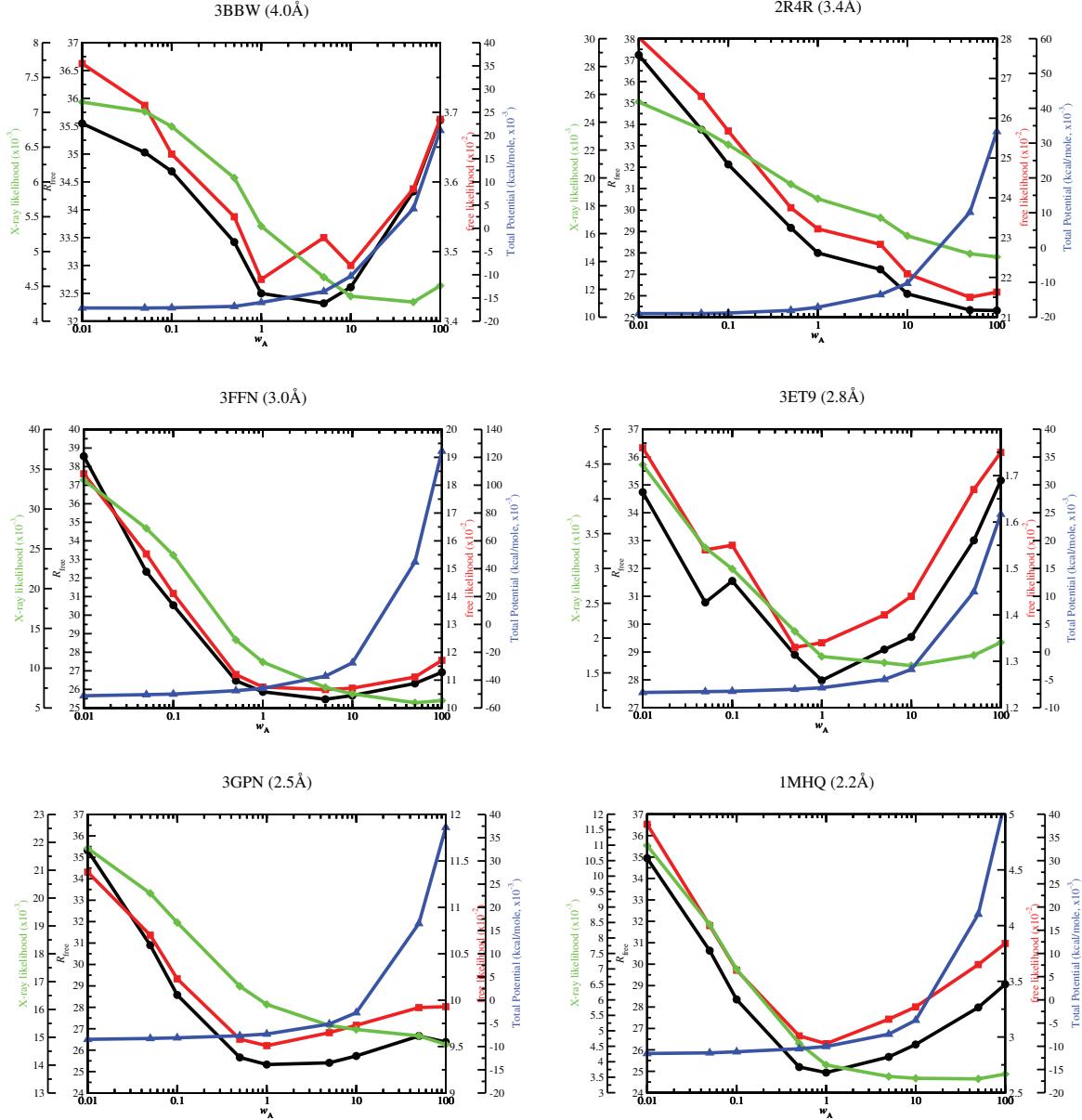


Figure 2: Plot of R_{free} (left Y axis, black), total X-ray potential (second left Y axis, green), X-ray free likelihood (right Y axis, red) and total chemical potential (second right Y axis, blue) versus w_A (logarithmic scale) for four representative structures ranging from 1.2 to 2.0 Å (PDB IDs and resolutions are given above each respective plot).

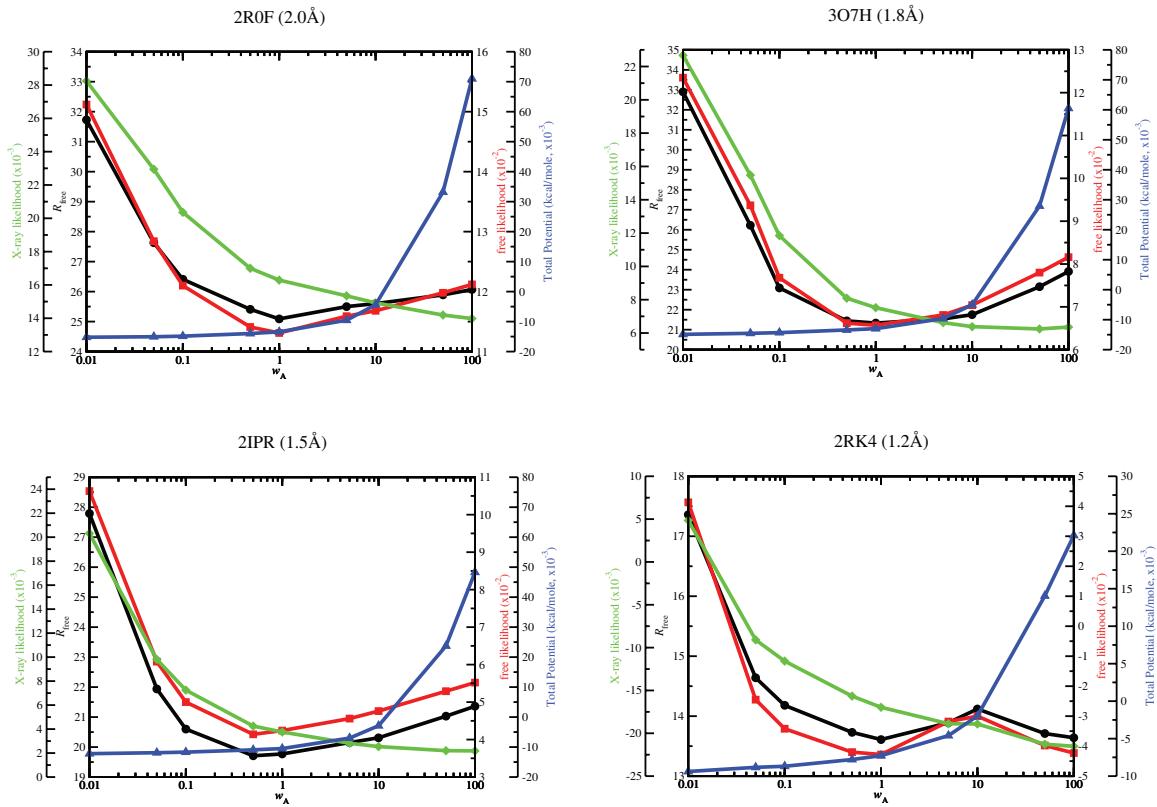


Figure 3: Detail of the hydrogen bond shown in Figure 5 with $2F_{\text{obs}} - F_{\text{calc}}$ electron density contoured at 1σ . A) Result from the phenix refinement and B) result from the FFX based refineemnt.

