Structural frameworks for considering microbial protein and nucleic-acid dependent motor ATPases Nathan D. Thomsen and James M. Berger



Figure S1. Nucleotide binding and quaternary organization of ABC ATPases

A. Topology diagram of the RecA-like core of the ABC ATPase fold. Conserved motifs, catalytic residues and secondary structural elements are coloured as in Figure 1. Locations of ABC inserts are marked with solid black triangles. Note the lack of helix α B and strand β 3 found in most RecA-like ATPases, but the presence of the C-terminal β -hairpin. Abbreviations: CE = catalytic glutamate, W-A = Walker A, W-B = Walker B, H = H loop, D = D loop, Q = Q loop, C = C region or ABC signature motif.

B. The active site of *Pyrococcus furiosus* Rad50 (PDB entry 1F2U) (Hopfner *et al.*, 2000) highlighting the location of catalytic residues common to ABC ATPases. The adjacent subunit, which contributes residues from the C and D motifs, is shown in dark grey. Active site elements are coloured as in Figure 1.

C. A dimer of two Rad50 (PDB entry 1F2U) (Hopfner *et al.*, 2000) nucleotide-binding domains illustrating the dual, bipartite active site formed by ABC ATPases. The two RecA-like folds are shown in yellow and cyan, with structural elements unique to the ABC family shown in grey. Active site residues contributed in *trans* to a partner catalytic centre (motifs C and D) are shown in coloured sticks and labelled.