Figure S4 The linker region (the dotted line) connecting C-terminus of the NBD and N-terminus of the TMD possibly accounts for the “beak” regions and the unmatched regions in the NBDs between the refined ABCG2 model and the ABCG2 map.
Figure S5  Shown is the sequence alignment between human ABCG2 and the two halves of murine ABCB1 (PDB code: 3G5U), illustrating the difference in intracellular loops (ICLs) between the two ABC transporters. ABCB1A* and ABCB1B* represent the first and second halves of ABCB1 and were created by cutting the ABCB1 protein sequence to two halves and then changing the order of TMD and NBD in order to get amino acid sequences that can be directly aligned with that of ABCG2. Amino acid identity and similarity were identified using the BLOSUM62 software and are highlighted with colors. Putative TM helices are highlighted with red lines above the sequences. Two coupling helices of each half of the ABCB1 molecule within the long ICLs that have direct contacts with the NBDs are highlighted with brown lines above the sequences. This sequence alignment suggests that, in contrast to ABCB1, each ABCG2 molecule contains only one long ICL with a potential coupling helix. This illustration is similar to what we previously published (Rosenberg et al., 2010).