Supplementary Information, Figure S3

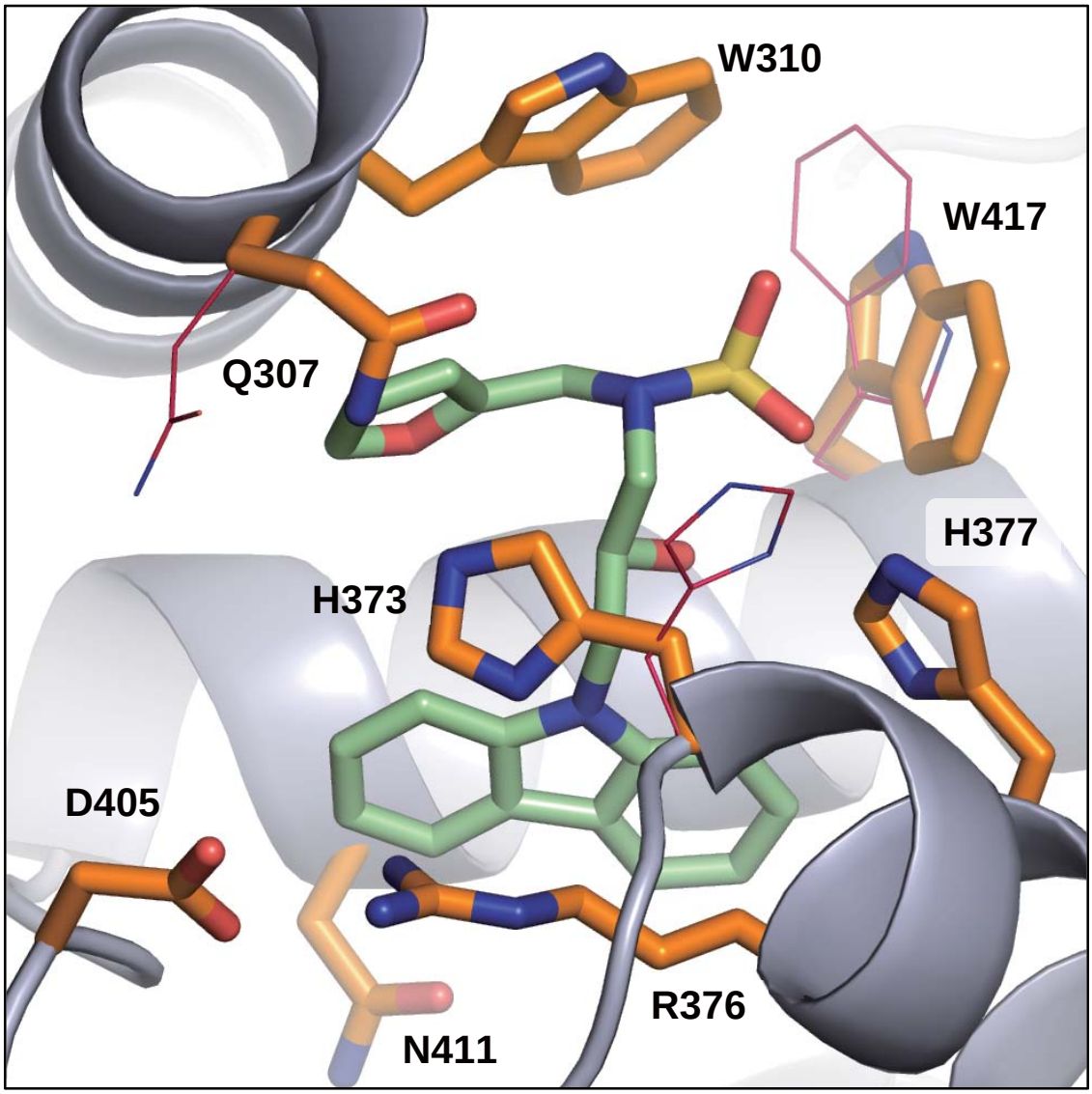

Figure S3. KL001-binding site on murine CRY2. A close view of the interactions between KL001 and CRY2 cofactor pocket residues. As a key structural component of the inner cleft, R376 and D405 form the characteristic salt-bridge within the FAD-binding pocket of cryptochromes and photolyases. Mutations of murine CRY1 D387 and N393 (mCRY2 D405 and N411, respectively) are known to abolish KL001 binding. KL001 binding is associated with side chain conformational changes in H373, Q307, and W417. The rotamers of these residues in apo CRY2 are shown in line representation and colored in pink. The methanesulfonamide group of KL001 is accommodated by an outer vestibule of the CRY2 FAD-binding pocket constructed by H377, W310, and W417.