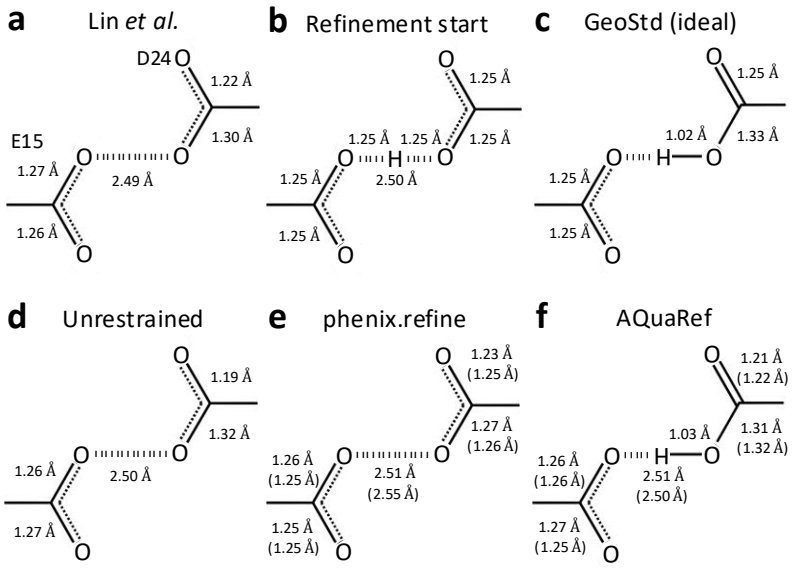

Figure X. Wild-type DJ-1 (PDB code: 5SY6). Bond distances in the moiety of hydrogen bond between Oε2 (E15) and Oδ2 (D24): **(a)** as measured in downloaded from PDB model, **(b)** starting geometry for all refinements (H is present only in AQuaRef refinement), **(c)** ideal library values in Phenix; geometry of –COOH or –COO groups is the same for Asp and Glu residues, **(d)** unrestrained and **(e)** restrained refinement with phenix.refine, **(f)** refinement with AQuaRef. Distances in parentheses correspond to refinement using resolution-truncated data at 2 Å. H atom is shown only if it was explicitly modelled (present in the PDB model file).

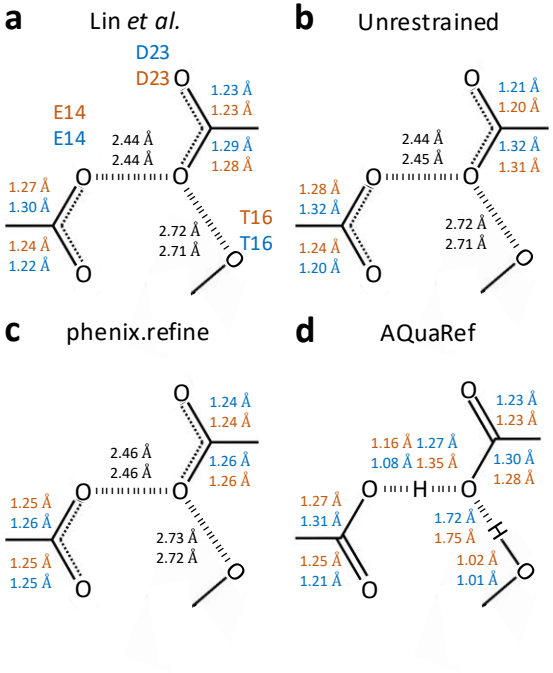

Figure Y. E. coli YajL (PDB code: 5SY4). Bond distances in the moiety of hydrogen bond between Oε2 (E14) and Oδ2 (D23) across chains A (blue) and B (orange): **(a)** as measured in downloaded from PDB model, **(b)** unrestrained and **(c)** restrained refinement using phenix.refine, **(d)** refinement with AQuaRef. H atom is shown only if it was explicitly modelled (present in the PDB model file).

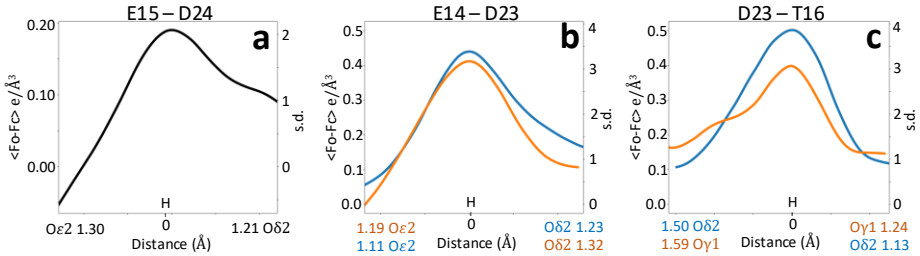

Figure Z. Mean values of the difference density map, shown in absolute units (e/Å³) and as standard deviation values along the O-H vector for the analyzed bonds for: (a) DJ-1 and (b-c) E. coli YajL models. All peak centers are aligned to the origin. Atoms belonging to chains A and B are shown in blue and orange, correspondingly.

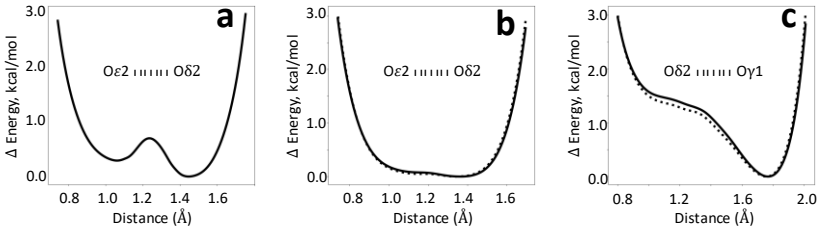

Figure W. AIMNet2 energy values relative to their minimum as a function of hydrogen position between corresponding oxygen atoms: (a) Oδ2 (D24) and Oε2 (E15) in DJ-1, (b) Oδ2 (D23) and Oε2 (E14) in YajL, and (c) Oδ2 (D23) and Oγ1 (T16) in YajL. Solid and dashed lines represent two instances of the bond in the YajL model.