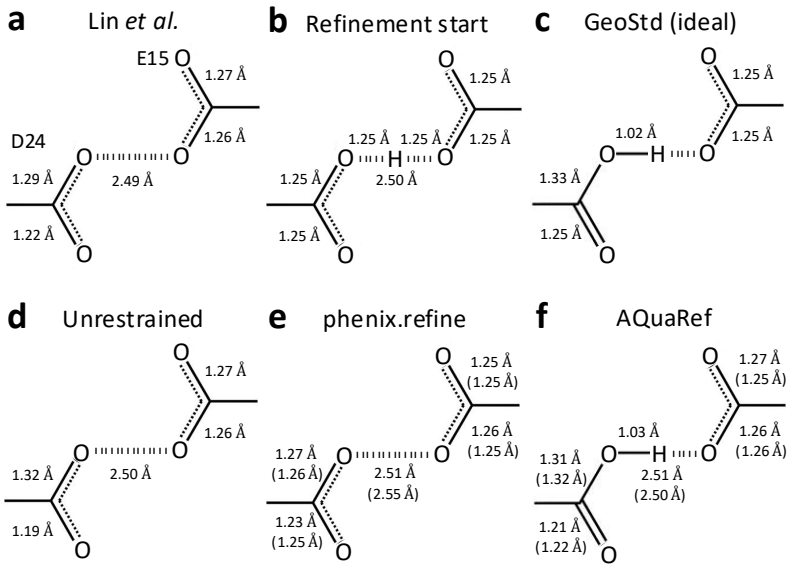

Figure X. Wild-type DJ-1 (PDB code: 5SY6). Bond distances in D24 and E15 moiety: **(a)** as in downloaded 5SY6 model, **(b)** starting geometry for all refinements (H is present only in AQuaRef refinement), **(c)** ideal library values in Phenix; geometry of –COOH or –COO groups is the same for Asp and 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).

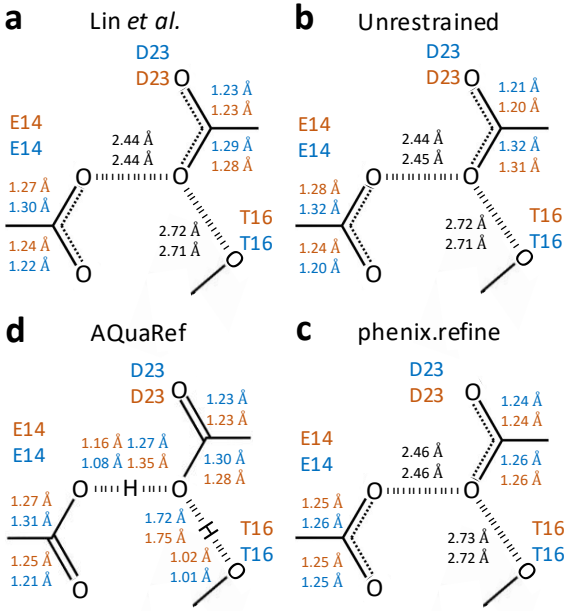

Figure Y. E. coli YajL (PDB code: 5SY4). Bond distances in D24 and E14 moiety across chains A (blue) and B (orange): **(a)** as in downloaded 5SY4 model, **(b)** unrestrained and **(c)** restrained refinement using Phenix, **(d)** refinement with AQuaRef. H atom is shown only if it was explicitly modelled (present in the PDB model file).

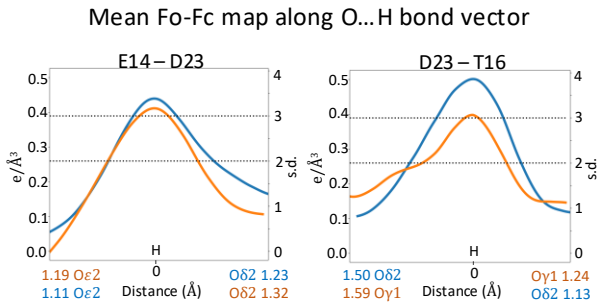

Figure Z. Mean values of the difference density map, shown in absolute units (e/Å³) and as r.m.s. deviation values along the O-H vector for the analyzed bonds for the E. coli YajL model (PDB code: 5SY4). The lower horizontal lines indicate the mean bulk solvent density (0.27 e/Å³) obtained from the flat bulk solvent model, the upper horizontal lines mark the 3 s.d. map level. All peak centers are aligned to the origin. Distances shown in orange and blue indicate distances between the map peak and corresponding oxygen atoms.

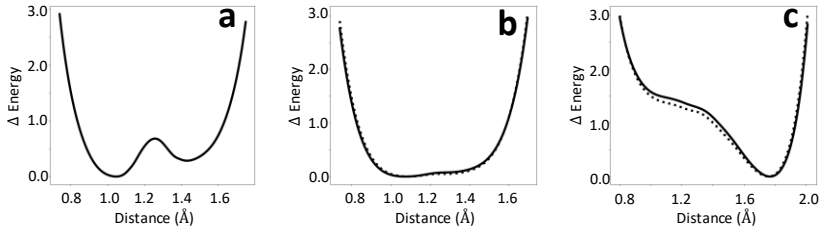

Figure W. AIMNet2 energy values relative to their minimum as a function of hydrogen position between corresponding oxygen atoms: (a) Oδ2 (D24) and Oε2 (E15) in 5SY6, (b) Oδ2 (D23) and Oε2 (E14) in 5SY4, and (c) Oδ2 (D23) and Oγ1 (T16) in 5SY4. Solid and dashed lines represent two instances of the bond in the model.