Engineered tryptophan in the adenine binding of catalytic subunit A of the A-ATP synthase demonstrates the importance of aromatic residues in adenine binding, forming a tool for steady state and time-resolved fluorescence spectroscopy

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Supplementary figure legend

Figure S1: Overlap of crystallographic structures of F427W mutant (*green*; PDB 3SDZ) with WT-A subunit (*orange*; PDB 3I72; Kumar *et al.*, 2010). An insert showing the flattened P-loop (G234-T241) in F427W mutant making a drift of around 6.8 Å in comparison to the arched conformation of the P-loop in WT-A. The drift was measured between the Cα atoms of G237 residue.

Figure S2: Structural overlap of AMP-PNP binding region within 5 Å in AMP-PNP bound structure of WT-A (yellow; PDB 3I4L; Kumar *et al.*, 2010) with F508W (*cyan*, PDB 3SEO) mutant structure of subunit A. The AMP-PNP molecule is shown as spheres (wheat colour). The mutated residue in F508W mutant is labelled as asterisk (*). For clarity the residues of AMP-PNP bound structure of subunit A are labelled.

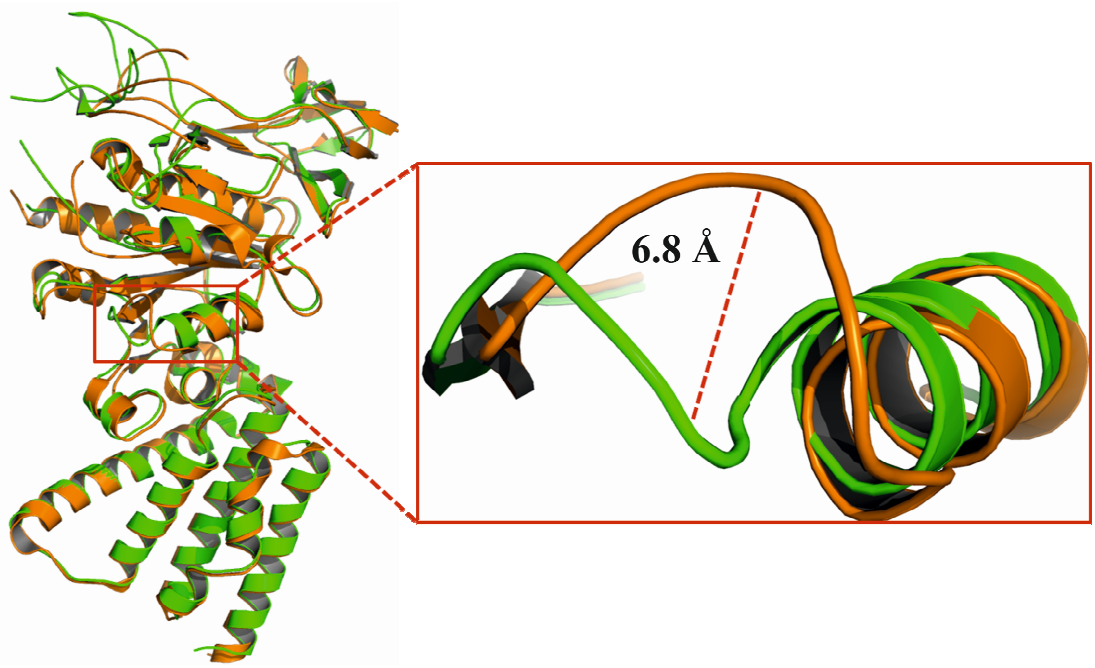

Figure S1

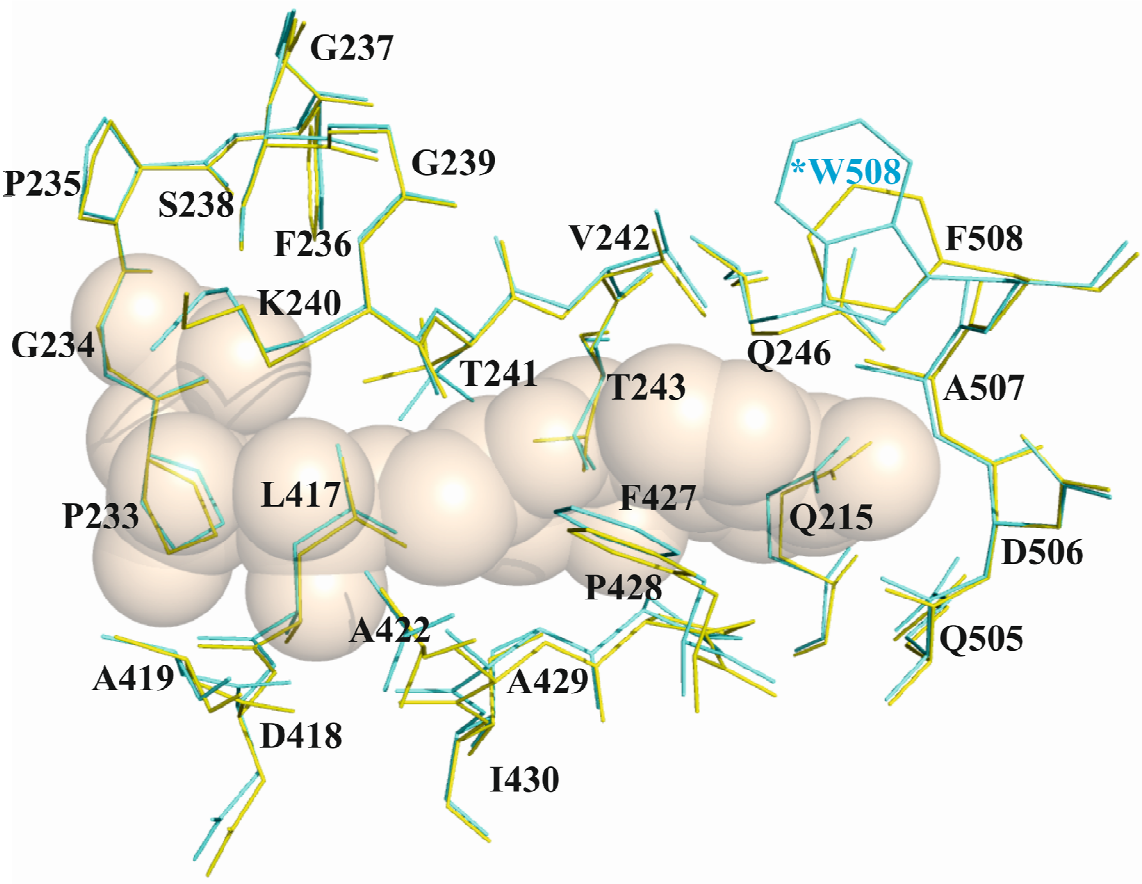
G237
P235
S238
G239
F236
*W508
V242
F508
K240
G234
T241
T243
Q246
A507
L417
P233
F427
Q215
D506
P428
A422
Q505
A419
A429
D418
I430

Figure S2