

**Supplementary Information for  
Guanine–aspartic acid interactions probed with IR–UV resonance spectroscopy**

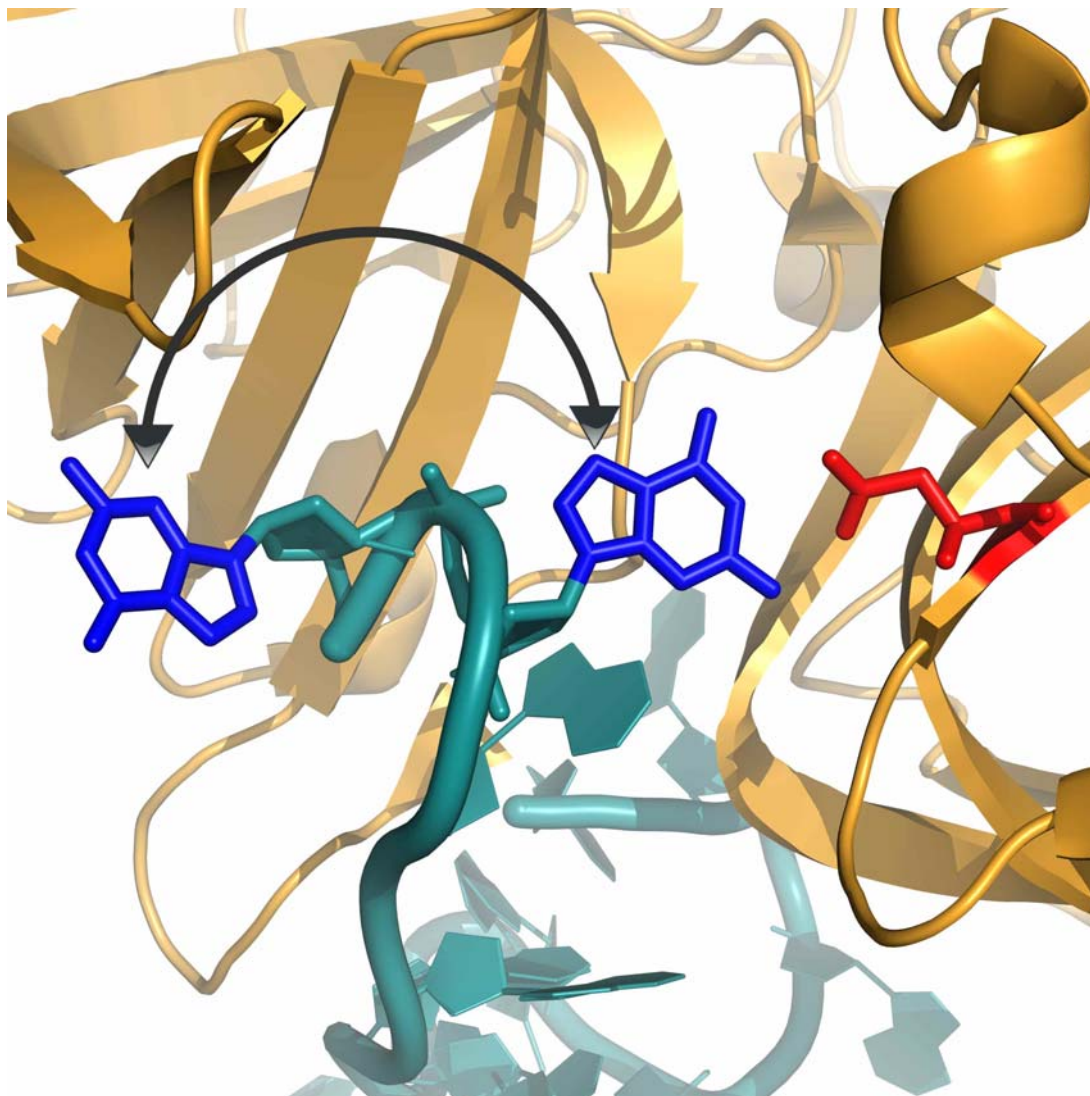


Figure S1. Picture of interaction between guanine and aspartic acid in pdb 1JB7. Guanine can adopt two different positions suggesting that it could serve as a molecular recognition agent.

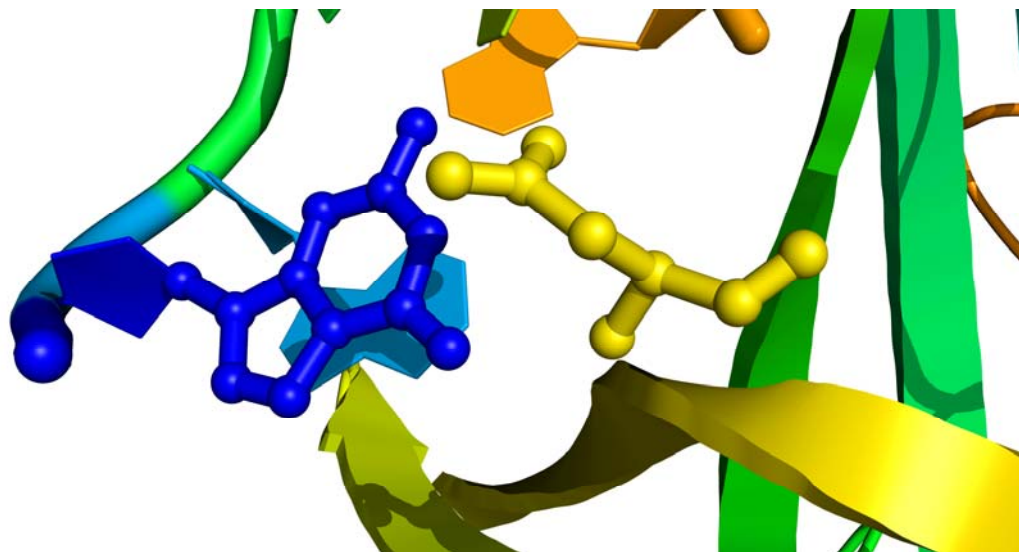
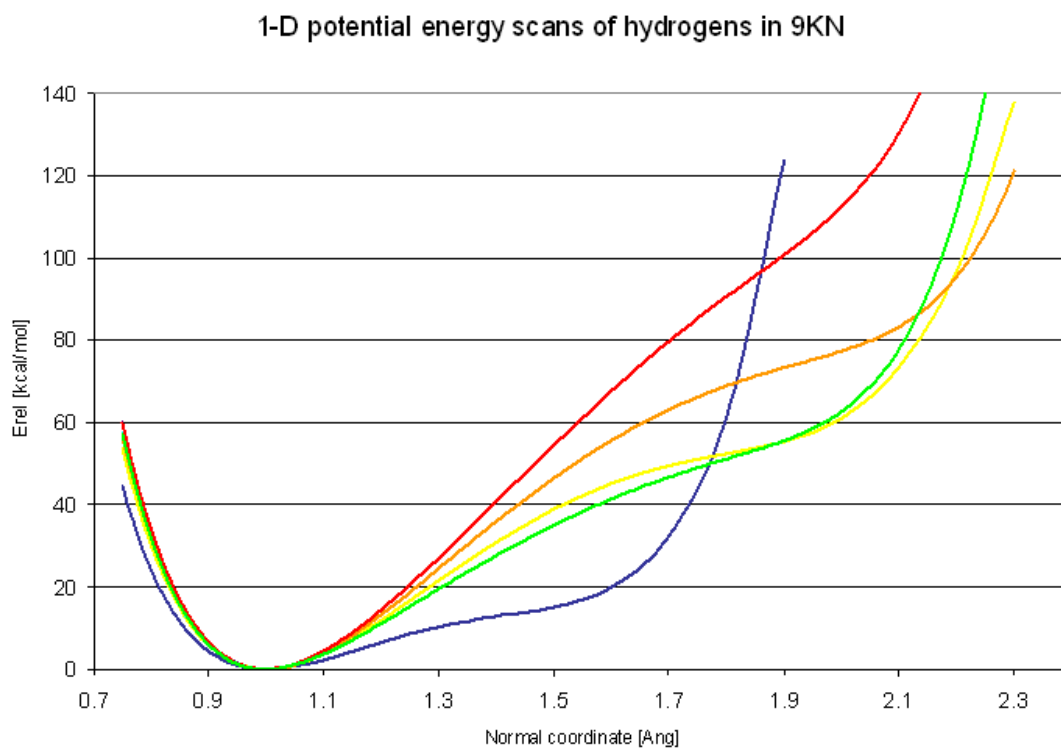


Figure S2. Sample interaction of aspartic acid and guanine in structure 1QZG. In this structure aspartic acid interacts via both the COOH and the C=O group, similarly to structures we obtained in vacuo.



**Figure S3:** One-dimensional potential energy scans of 5 hydrogens in 9KN. Colours of individual scans corresponds to 9KN structure colouring in figure 3 in the text: red curve corresponds to N9H on guanine, yellow to N3H<sub>HB</sub> on guanine, orange to the NH<sub>2</sub> symmetrical stretch on guanine, blue to COOH<sub>HB</sub> on the R group of the aspartic acid and green to COOH on the C-terminus of the aspartic acid.