

# **PSAP: Protein Structure Analysis Package**

## **Supplementary Figures**

**B. Balamurugan<sup>1</sup>, M.N.A. Md. Roshan<sup>1</sup>, B. Shaahul Hameed<sup>1</sup>,  
K. Sumathi<sup>1</sup>, R. Senthil Kumar<sup>1</sup>, A. Udayakumar<sup>1</sup>,  
K.H. Venkatesh Babu<sup>1</sup>, M. Kalaivani<sup>1</sup>, G. Sowmiya<sup>1</sup>, P.  
Sivasankari<sup>1</sup>, S. Saravanan<sup>1</sup>, C. Vasuki Ranjani<sup>1</sup>,  
K. Gopalakrishnan<sup>1</sup>, K.N. Selvakumar<sup>1</sup>, M. Jaikumar<sup>1</sup>,  
T. Brindha<sup>1</sup>, Daliah Michael<sup>1</sup> and K. Sekar<sup>1,2,\*</sup>**

<sup>1</sup>Bioinformatics Centre  
(Centre of Excellence in Structural biology and Bio-computing)

<sup>2</sup>Supercomputer Education and Research Centre  
Indian Institute of Science  
Bangalore 560 012, India

\*To whom correspondence should be addressed

E-mail: sekar@physics.iisc.ernet.in and sekar@serc.iisc.ernet.in

Phone: +91-080-22933059/22932469/23601409

Fax: +91-080-23600683 and 23600551

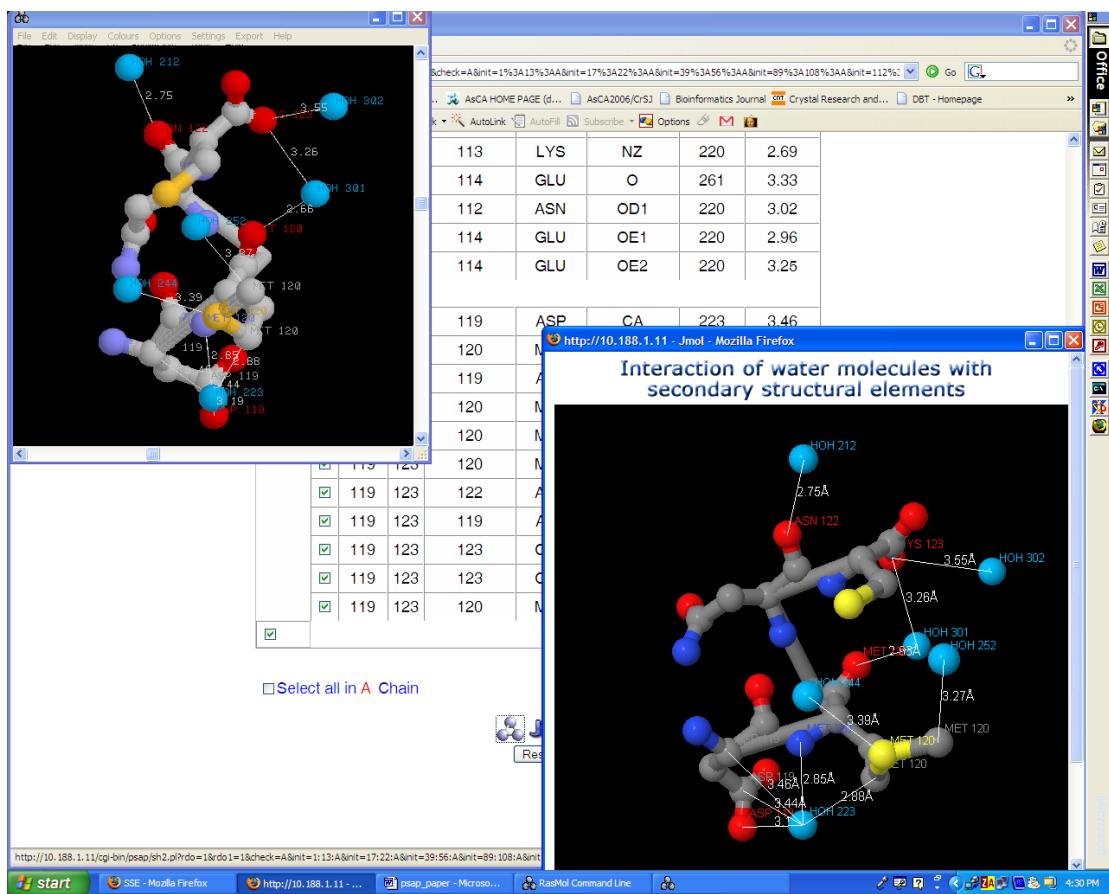
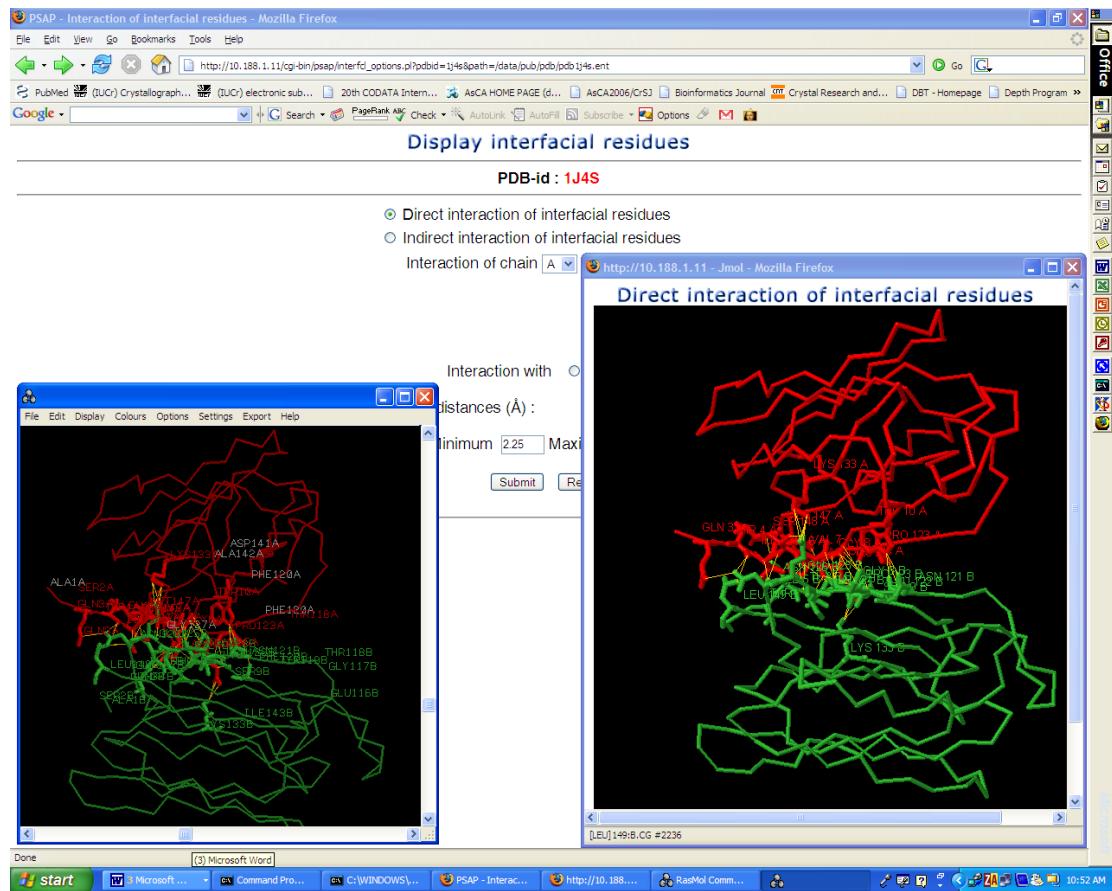


Figure S1. The interaction of water molecules with a particular helix (residues 119-123). As can be seen, six water molecules are involved in the interaction. The PDB-id of the structure is 1GH4.



**Figure S2.** The output panel depicts the direct interaction of the interfacial residues at the dimer interface of the subunits A and B (1J4S). The subunits A and B are shown in red and green colors respectively.

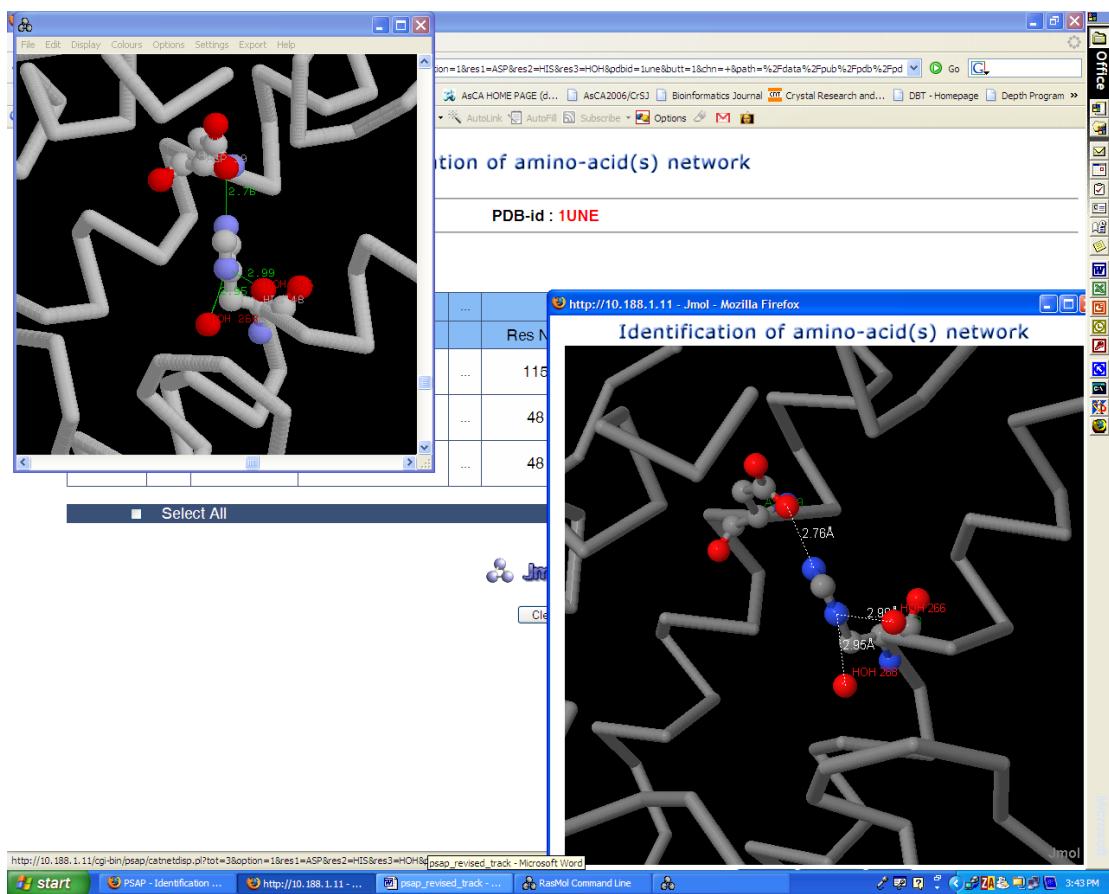


Figure S3. The screen snapshot shows the catalytic network formed by the residues Aspartate and Histidine and a water molecule (PDB-id: 1UNE).