|  |  |  |  |
| --- | --- | --- | --- |
| **Compounds** | **Hydrogen bonds** | **Hydrophobic interactions** | **ΔGb (Kcal/mol)** |
| **Quercetin** | **Ser-A222, Asn-A252, Asn-A258, Thr-A306, Thr-C306** | **Ile-A221, Val-A299** | **- 8.1** |
| **5-Hydroxyflavone** | **Thr-C306, Asn-A252** | **Ile-A221, Val-A299** | **-6.7** |
| **Rutin** | **n.e.d\*** | **n.e.d\*** | **n.e.d\*** |

Table 1

The stereochemical quality of the final structures (i.e. the distribution of phy and psi angles) were assessed by means of the PROCHECK program [Laskowski RA et al. 1993]. With this test, no severely disallowed atomic contacts were detected, suggesting essentially good stereochemistry, with 88.2-88.5 % and 98.8 % of the amino acids residues in the most favoured and additionally allowed regions, respectively and with 2- 1.9 % and 0.8 % residues in generously allowed and disallowed regions of the Ramachandran plot



Ramachandran plot of closed state model.

 Ramachandran plot of open state model.



The G loop area: the open state in magenta, the closed state in green