PIC : Protein Interaction Calculator

CRITERIA FOR RECOGNIZING VARIOUS TYPES OF INTERACTIONS

1. HYDROPHOBIC INTERACTIONS:

The following residues are considered to participate in interactions if they fall within 5Å range.
ALA, VAL, LEU, ILE, MET, PHE, TRP, PRO, TYR.
Reference: Kyte and Doolittle.

2. DISULPHIDE BRIDGES:

Pairs of cysteines (sulphur atoms) within 2.2 Å are considered as disulphide bridges.

3. HYDROGEN BOND :

Criteria for hydrogen bond definition :-
donor-acceptor distance cutoff (oxygen and nitrogen) = 3.50
donor-acceptor distance cutoff (sulphur) = 4.00
Reference: J. Overington, et al. *Proc. Roy. Soc. Biol Sci.* 1990, pg.132-145

4. IONIC INTERACTIONS:

Ionic residue(ARG,LYS,HIS,ASP,GLU) pairs falling with 6Å (default) contribute to ionic interactions.

5. AROMATIC-AROMATIC INTERACTIONS:

Pairs of phenyl ring centroids that are seperated by a preferential distance of between 4.5 to 7 Å account for aromatic interactions.
Reference: S.K.Burley, G.A.Petsko, *Science*, 1985, Vol 299, pg.23-28.

6. AROMATIC-SULPHUR INTERACTIONS:

Interactions between the sulphur atoms of cysteine and methionine and the aromatic rings of phenylalanine, tyrosine and tryptophan within 5.3 Å account for aromatic-sulphur interactions.
Reference: K.S.C Reid, P.F.Lindley and J.M. Thornton, *FEBS letter* 1985, Vol.190, pg.209-213.

7. CATION-PI INTERACTIONS:

When a cationic side chain (Lys or Arg) is near an aromatic side chain (Phe, Tyr, or Trp) within 6 Å separation they account for cation-pi interactions.
Reference: R.Satyapriya and Saraswathi Vishveshwara, *Nucleic Acid Research* , 2004, Vol 32, pg.4109-4118.

8. SOLVENT ACCESSIBILITY:

To calculate the total accessible surface area of a protein NACCESS program is used.
Residues that has a total relative accessibility value greater than 7 are considered as exposed.
Residues that has a total relative accessibility value less than or equal to 7 are considered as buried.
Reference: S.J. Hubbard, & J.M. Thornton, 'NACCESS'. 1993. (VERSION 2.1.1).

9. DEPTH CALCULATION:

Atoms near surface are recognised with residue depth value less than or equal to 5.
Reference: Suvobrata Chakravarty and Raghavan Varadarajan, *Structure*, 1999, Vol 7, Pg.723–732.