- Evaluate solvent accessible surface area (SASA) of a central strand within an amyloid fibril (Folded state).
- Evaluate SASA of isolated, extended strand using an approximation (Reference state). That is, for residue n, evaluate SASA for the isolated tripeptide in the absence of side chains on n-1 and n+1.
- Take the difference, $SASA_{Ref}$ –$SASA_{Fold}$ for each atom to get area buried.
- Multiply the area buried by the Atomic Solvation Parameter (ASP).

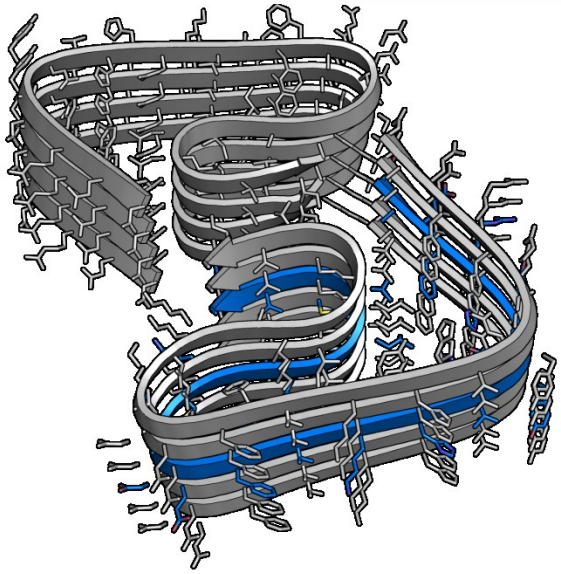
```
     +18 cal/mol/Å² for C
      -5 cal/mol/Å² for S
      -9 cal/mol/Å² for N,O uncharged
-38,-37 cal/mol/Å² for N,O charged
```

Except in the following cases:

1. ASP=0 for **Asn** or **Gln** side chains N and O elements with two-H-bonds and less than 5 Å² SASA.
2. ASP=0 for backbone N and O elements involved in H-bond.
3. ASP>-9 for ionizable N or O elements involved in ion pair and less than 50 Å² SASA. Ion pair distance must be less than 4.5 Å. ASP depends on distance as follows: A.S.P. =-9* ((dist-2.8Å)/2.8Å)² .
4. Include entropy terms from Koehl & Delarue 1994 scaled by percentage of side chain surface area buried.

- Sum up the energies of all the atoms to get the solvation energy. Negate this value to get stabilization energy.
- Less sensitive to structural errors than Rosetta.

Folded state



Reference state

Eisenberg D, Wesson M, Yamashita M (1989) Interpretation of protein folding and binding with atomic solvation parameters. Chemica Scripta 29A: 217–221.
Koehl P, Delarue M. Application of a self-consistent mean field theory to predict protein side-chains conformation and estimate their conformational entropy. J Mol Biol. 1994 Jun 3;239(2):249-75.