

Instruction on how to submit a PDB pool

- 1- The PDB pool file should be saved as a “.txt” and the user needs to have access to the URL of the PDB pool (i.e. <http://www.stat.tamu.edu/~madoliat/LagSVD/pdb-p.txt>).
- 2- The line starts with `#` is considered as a remark line and it will not be interpreted by the LagSVD web-tool.
- 3- The colon symbol `:` is used for separation of the different fields.
- 4- Each row contains the information of an amino acid as follows:
 - a. Protein name: is a consistent name used to indicate the protein name of the amino acids.
 - b. Model: is set to be 1 in LagSVD v0.10.
 - c. Chain: is set to be A in LagSVD v0.10.
 - d. Number: indicates the position of the amino acid in the sequence (It should be right adjusted in a four characters word).
 - e. Ins: can be filled by indicating the secondary structure.
 - i. 0: α -helix 1: β -sheet 2: coil
 - f. Type: three letters words for the amino acid.
 - g. η (θ , ϕ , ...): the first element of the pair of the dihedral/planar angles.
 - h. ζ (τ , ψ , ...): the second element of the pair of the dihedral/planar angles.