Instruction to use D2N tool

D2N is a tool for calculating the distance of modeled protein structure without using its corresponding experimental native structure. This tool unable us to predict the quality of modeled structure, result is reported as different parameters such as RMSD, TM and GDT.

Query sample file:

 ➢ Only PDB protein file id accepted (No DNA-Protein, Ligand-Protein etc).
 ➢ No header section is required; PDB file should have only co-ordinates information.
 ➢   Example: sample.pdb

```
ATOM      1   N    MET      1      81.063   38.998   43.300   1.00   0.00
ATOM      2   H1   MET      1      81.682   39.176   44.076   1.00   0.00
ATOM      3   H2   MET      1      80.273   39.632   43.412   1.00   0.00
ATOM      4   H3   MET      1      81.497   39.227   42.420   1.00   0.00
ATOM      5   CA   MET      1      80.556   37.616   43.319   1.00   0.00
ATOM      6   HA   MET      1      79.788   37.530   42.551   1.00   0.00
ATOM      7   CB   MET      1      81.651   36.566   43.057   1.00   0.00
ATOM      8  2HB   MET      1      82.322   36.512   43.916   1.00   0.00
ATOM      9  3HB   MET      1      81.170   35.594   42.944   1.00   0.00
ATOM     10   CG   MET      1      82.505   36.832   41.812   1.00   0.00
```

Result:

 ➢ RMSD: root mean square deviation is an important parameter for estimating the distance between two superimposed structures. It usually expressed in Å. Here RMSD is predicted for uploaded structure to access the quality of modeled structure.

 ➢ TM: template modeling score or TM-score is a measure of similarity between two protein structures with different tertiary structures. This score lie between (0,1], where lower value represents poor quality whereas high value represents good quality structure.

 ➢ GDT: The global distance test (GDT), also written as GDT TS to represent "total score", is a measure of similarity between two protein structures with identical amino acid sequences but different tertiary structures. Here again lower value represents poor quality whereas high value represents good quality structure.

Once job is submitted a job ID would be created (ex: "6981038d2n"). As the result is not immediate so user are requested to note this job ID which they can enter in future to get the status. Alternative way to receive result is via email. If user provides email ID then he/she will get result on email ID as a web link (ex: http://www.scfbio-iitd.res.in/software/69810638d2n). By following this link user can see the final result example of result is shown below:

Distance To Native Result

Structure Name	RMSD (Ang)	TM	GDT
Bilab-ENABLE_TS3.pdb	10.77	0.49	0.42

Physicochemical Parameters of Protein

PDB Name	Area	Eucledian Distance	Energy (Kcal/mol)	Secondary Structure Panelty	Residue Length	CB Pair Number
Bilab-ENABLE_TS3.pdb	9969.93	25892.9	571504	42	166	1111

Thank you for using D2N Tool
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