

**Fig. 3**

```
<dock_design>
<TASKOPERATIONS>
  <InitializeFromCommandline name=IFC/> # use the information in the args file to supplement this XML
  <IncludeCurrent name=IC/> # includes the rotamers in the input structure (may not want to use)
  <RestrictDesignToProteinDNAInterface name= Dnalnt base_only =1 z_cutoff =6.0 dna_defs =Z.409.GUA/> #
  make the target site substitution of interest (chainID.crystalposition.type) and designate the sphere of residues
  surrounding it that are designable and packable
    <OperateOnCertainResidues name=AUTOprot> # works with the Dnalnt operation to enable residues to be
  chosen for design and packing if they are marked as AUTO
    <AddBehaviorRLT behavior=AUTO/>
    <ResidueHasProperty property=PROTEIN/>
  </OperateOnCertainResidues>
</TASKOPERATIONS>
<SCOREFXNS>
  <DNA weights=optimizedenergyfxn/> # energy function for design evaluation, this file must be put in the
  directory (ie, rosetta_database/scoring/weights/optimizedenergyfxn.wts)
</SCOREFXNS>
<FILTERS>
  <FalseFilter name=falsefilter/> # RosettaScripts has the ability to only output designs that pass a designated
  filter. This functionality is not being used here.
</FILTERS>
<MOVERS>
  <DnaInterfacePacker name=DnaPack scorefxn=DNA task_operations=IFC,IC,AUTOprot,Dnalnt/>
</MOVERS>
<PROTOCOLS>
  <Add mover_name=DnaPack/>
</PROTOCOLS>
</dock_design>
```