

</ROSETTASCRIPTS>

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<SCOREFXNS>
  <ScoreFunction name="ligand_soft_rep" weights="ligand_soft_rep">
    <Reweight scortype="fa_clec" weight="0.42" />
    <Reweight scortype="hbond_bb_sc" weight="1.3" />
    <Reweight scortype="hbond_sc" weight="1.3" />
    <Reweight scortype="rama" weight="0.2" />
  </ScoreFunction>
  <ScoreFunction name="hard_rep" weights="ligand">
    <Reweight scortype="fa_intra_rep" weight="0.004" />
    <Reweight scortype="fa_clec" weight="0.42" />
    <Reweight scortype="hbond_bb_sc" weight="1.3" />
    <Reweight scortype="hbond_sc" weight="1.3" />
    <Reweight scortype="rama" weight="0.2" />
  </ScoreFunction>
</SCOREFXNS>

<LIGAND_AREAS>
  <LigandArea add_nbr_radius="true" all_atom_mode="true" chain="X" cutoff="6.0" name="inhibitor_dock_sc" />
  <LigandArea add_nbr_radius="true" all_atom_mode="true" chain="X" cutoff="6.0" name="inhibitor_final_sc" />
  <LigandArea Alpha_restraints="0.3" add_nbr_radius="false" all_atom_mode="true" chain="X" cutoff="7.0" name="inhibitor_final_bb" />
</LIGAND_AREAS>

<INTERFACE_BUILDERS>
  <InterfaceBuilder ligand_areas="inhibitor_dock_sc" name="side_chain_for_docking" />
  <InterfaceBuilder ligand_areas="inhibitor_final_sc" name="side_chain_for_final" />
  <InterfaceBuilder extension_window="3" ligand_areas="inhibitor_final_bb" name="backbone" />
</INTERFACE_BUILDERS>

<MOVEMAP_BUILDERS>
  <MoveMapBuilder minimize_water="false" name="docking" sc_interface="side_chain_for_docking" />
  <MoveMapBuilder bb_interface="backbone" minimize_water="false" name="final" sc_interface="side_chain_for_final" />
</MOVEMAP_BUILDERS>

<SCORINGGRIDS ligand_chain="X" width="30">
  <ClassicGrid grid_name="classic" weight="1.0" />
</SCORINGGRIDS>

<TASKOPERATIONS>
  <TASKOPERATIONS>
    <MOVERS>
      <StartFrom chain="X" name="start_from">
        <Coordinates x="176.0032" y="222.4581" z="148.5608" /><Coordinates x="193.4029" y="229.3899" z="109.4270" /></StartFrom>
      <Transform angle="20" box_size="14" chain="X" cycles="1000" initial_perturb="5.0" move_distance="0.2" name="transform" repeats="1" temperature="5" />
      <HighResDocker cycles="6" movemap_builder="docking" name="high_res_docker" repack_every_nth="3" scorefxn="ligand_soft_rep" />
      <FinalMinimizer movemap_builder="final" name="final" scorefxn="hard_rep" />
      <InterfaceScoreCalculator chains="X" name="add_scores" scorefxn="hard_rep" />
    </MOVERS>
    <PROTOCOLS>
      <Add mover_name="start_from" />
      <Add mover_name="transform" />
      <Add mover_name="high_res_docker" />
      <Add mover_name="final" />
      <Add mover_name="add_scores" />
    </PROTOCOLS>
  </TASKOPERATIONS>
</TASKOPERATIONS>

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