
Supplementary information

**Structure and receptor recognition by the
Lassa virus spike complex**

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Supplementary Data for:

Structure and Receptor Recognition by the Lassa Virus Spike Complex

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This file contains:

Supplementary methods.

Supplementary methods:

Command line for Rosetta modeling

```
rosetta_scripts_executable -database path_to_rosetta_database -parser:protocol  
thread_and_score.xml -out:suffix _window_sequence -s template_pdb -parser:script_vars  
cst_full_path=path_to_Ca_coordint_constraints start_position_A=3A start_position_B=3B  
start_position_C=3C seq_to_thread=window_sequence  
span_starts=3A,3B,3C,428a,428b,428c span_ends=24A,24B,24C,448a,448b,  
448c span_oris=in2out,in2out,in2out,out2in,out2in,out2in -nstruct 10
```

Where thread_and_score.xml is the RosettaScripts XML at the bottom; window sequence is the sequence to model; 3A,3B, 3C and 24A, 24B and 24C are the start and end positions of the TM to model in the PDB, respectively; 428a,428b and 428c are the start positions for the GP TM. and the span_oris parameter are the orientations of all six spans with respect to the membrane.

```
<ROSETTASCRIPTS>  
<SCOREFXNS>  
  <ScoreFunction name="full" weights="ref2015_memb">  
    <Reweight scoretype="coordinate_constraint" weight="0.64"/>  
    <Reweight scoretype="res_type_constraint" weight="0.5"/>  
  </ScoreFunction>  
  <ScoreFunction name="soft" weights="ref2015_soft">  
    <Reweight scoretype="mp_res_lipo" weight="1"/>  
    <Reweight scoretype="coordinate_constraint" weight="0.64"/>  
    <Reweight scoretype="res_type_constraint" weight="0.5"/>  
  </ScoreFunction>  
</SCOREFXNS>  
<TASKOPERATIONS>  
  <InitializeFromCommandline name="init"/>  
  <RestrictToRepacking name="rtr"/>  
</TASKOPERATIONS>  
<MOVERS>  
  <SimpleThreadingMover name="thread_A" start_position="%%start_position_A%%"  
thread_sequence="%%seq_to_thread%%" scorefxn="full"/>  
  <SimpleThreadingMover name="thread_B" start_position="%%start_position_B%%"  
thread_sequence="%%seq_to_thread%%" scorefxn="full"/>  
  <SimpleThreadingMover name="thread_C" start_position="%%start_position_C%%"  
thread_sequence="%%seq_to_thread%%" scorefxn="full"/>  
  <AddMembraneMover name="add_memb" membrane_core="10" steepness="4"  
span_starts_num="%%span_starts%%" span_ends_num="%%span_ends%%"  
span_orientations="%%span_oris%%"/>  
  <PackRotamersMover name="soft_repack" scorefxn="soft" task_operations="init,rtr"/>  
  <PackRotamersMover name="hard_repack" scorefxn="full" task_operations="init,rtr"/>  
  <RotamerTrialsMinMover name="RTmin" scorefxn="full" task_operations="init,rtr"/>  
  <MinMover name="soft_min" scorefxn="soft" chi="1" bb="1" jump="0"/>  
  <MinMover name="hard_min" scorefxn="full" chi="1" bb="1" jump="0"/>
```

```
<ConstraintSetMover name="add_CA_cst" cst_file="%%cst_full_path%%"/>
<ParsedProtocol name="refinement_block"> #10 movers
  <Add mover_name="soft_repack"/>
  <Add mover_name="soft_min"/>
  <Add mover_name="soft_repack"/>
  <Add mover_name="hard_min"/>
  <Add mover_name="hard_repack"/>
  <Add mover_name="hard_min"/>
  <Add mover_name="hard_repack"/>
  <Add mover_name="RTmin"/>
  <Add mover_name="RTmin"/>
  <Add mover_name="hard_min"/>
</ParsedProtocol>
<LoopOver name="iter4" mover_name="refinement_block" iterations="4"/>
</MOVERS>
<FILTERS>
  <Time name="timer"/>
</FILTERS>
<PROTOCOLS>
  <Add filter="timer"/>
  <Add mover="add_memb"/>
  <Add mover="add_CA_cst"/>
  <Add mover="thread_A"/>
  <Add mover="thread_B"/>
  <Add mover="thread_C"/>
  <Add mover="iter4"/>
  <Add filter="timer"/>
</PROTOCOLS>
<OUTPUT scorefxn="full"/>
</ROSETTASCRIPTS>
```