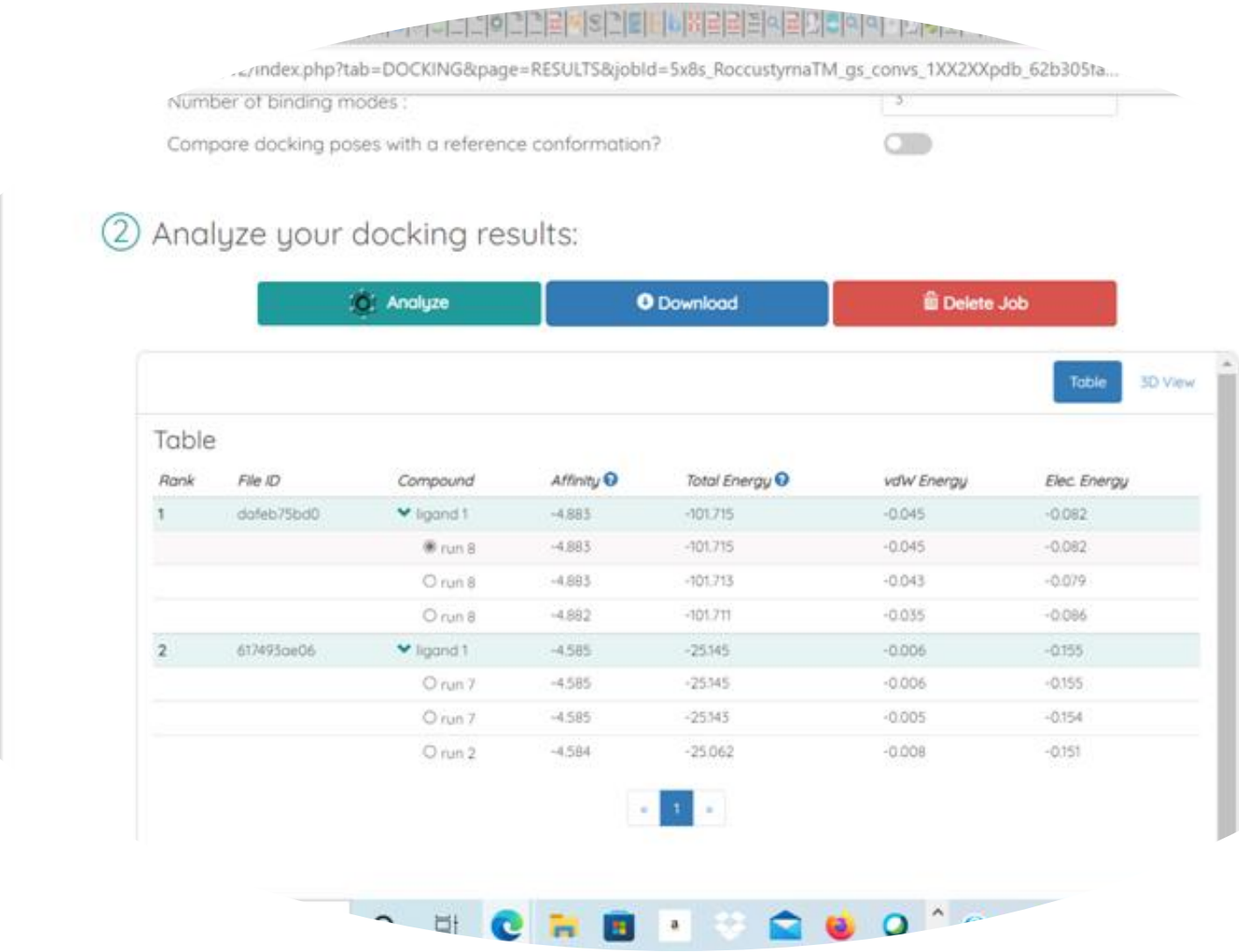
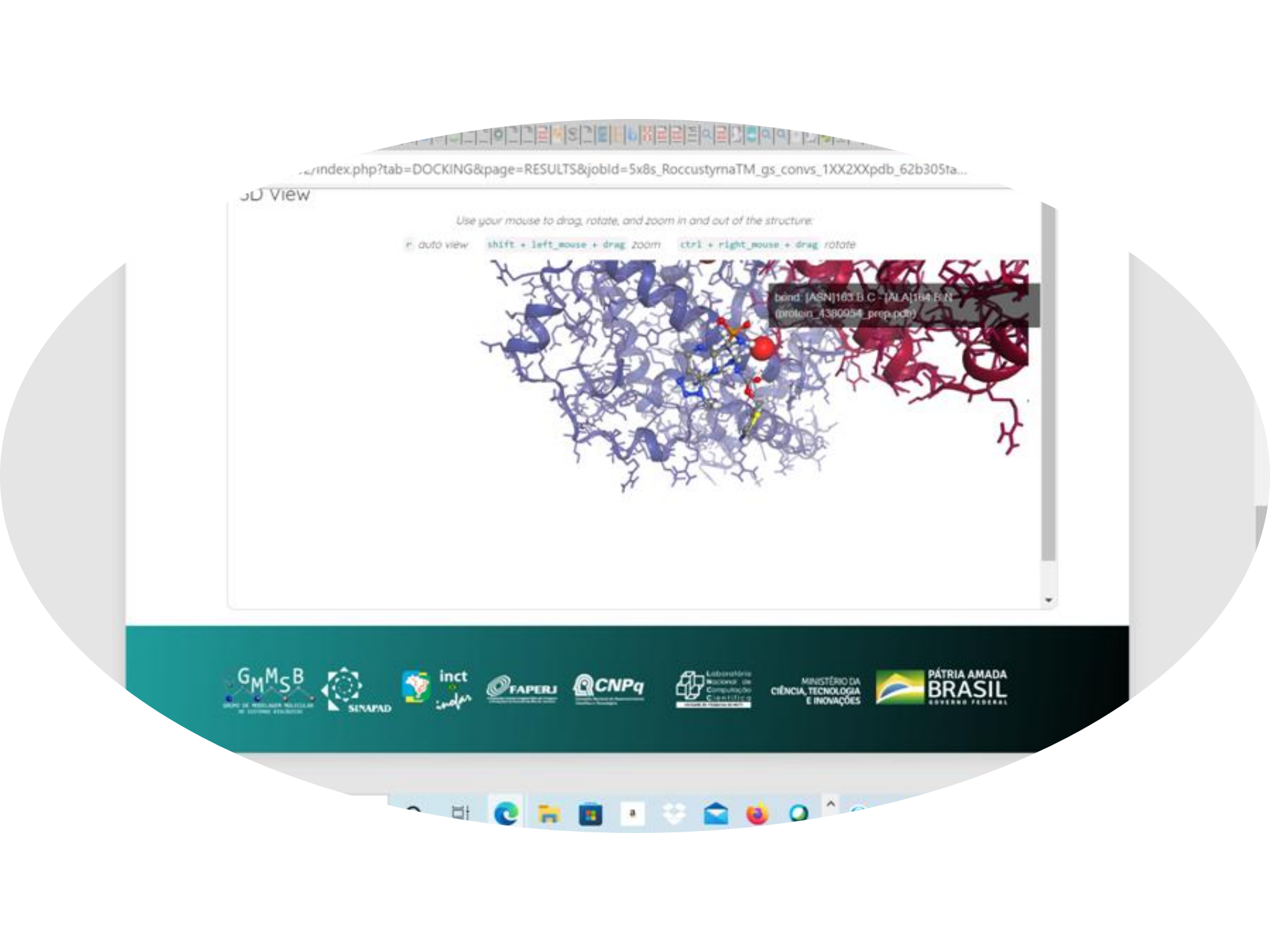

index.php?tab=DOCKING&page=RESULTS&jobId=5x8s_RoccustyrnaTM_gs_convs_1XX2XXpdb_62b305ta...
Number of binding modes :
Compare docking poses with a reference conformation?
② Analyze your docking results:
Analyze
Download
Delete Job
Table
3D View
Table
Rank File ID Compound Affinity Total Energy vdW Energy Elec. Energy
1 dafeb75bd0 ligand 1 -4.883 -101.715 -0.045 -0.082
run 8 -4.883 -101.715 -0.045 -0.082
run 8 -4.883 -101.713 -0.043 -0.079
run 8 -4.882 -101.711 -0.035 -0.086
2 617493ae06 ligand 1 -4.585 -25.145 -0.006 -0.155
run 7 -4.585 -25.145 -0.006 -0.155
run 7 -4.585 -25.143 -0.005 -0.154
run 2 -4.584 -25.062 -0.008 -0.151
1


index.php?tab=DOCKING&page=RESULTS&jobId=5x8s_RoccustyrnaTM_gs_convs_1XX2XXpdb_62b305ta...
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r: auto view
shift + left_mouse + drag: zoom
ctrl + right_mouse + drag: rotate
bond: [ASN]163:B.C - [ALA]164:B.N
(protein_4380954_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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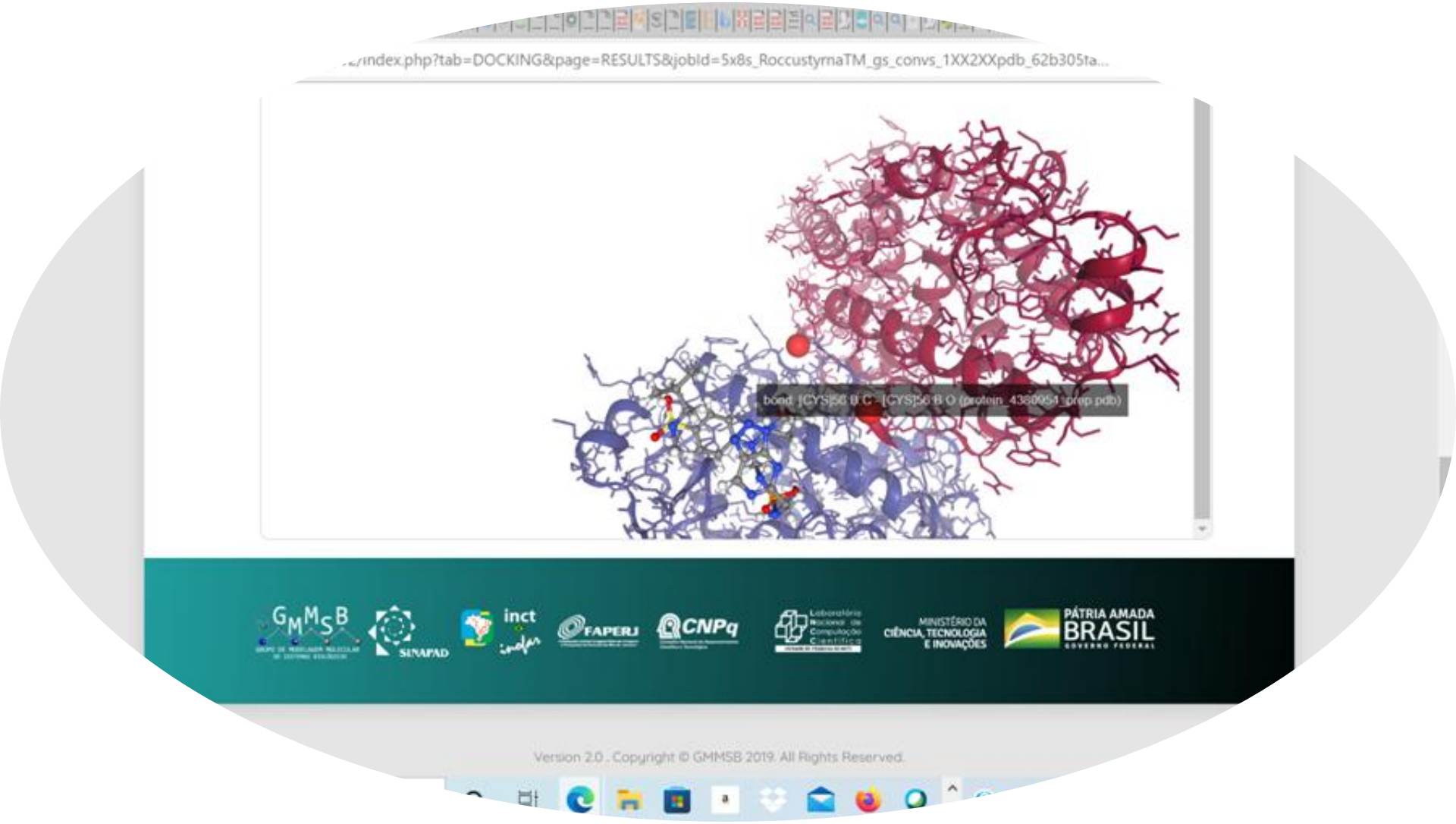
index.php?tab=DOCKING&page=RESULTS&jobId=5x8s_RoccustyrnaTM_gs_convs_1XX2XXpdb_62b305fa...
bond: [CYS]56 B C - [CYS]56 B O (protein_4380954_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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