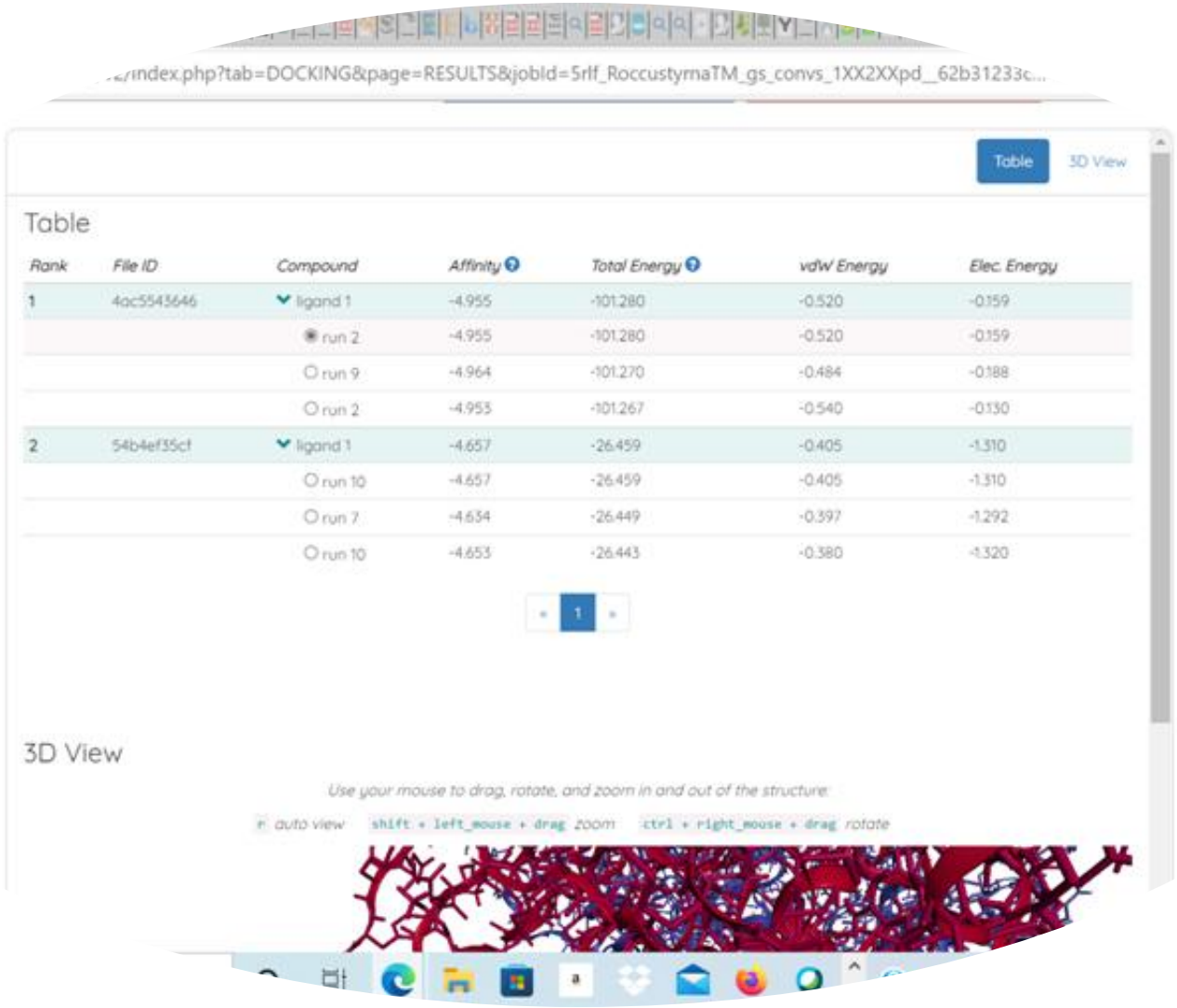
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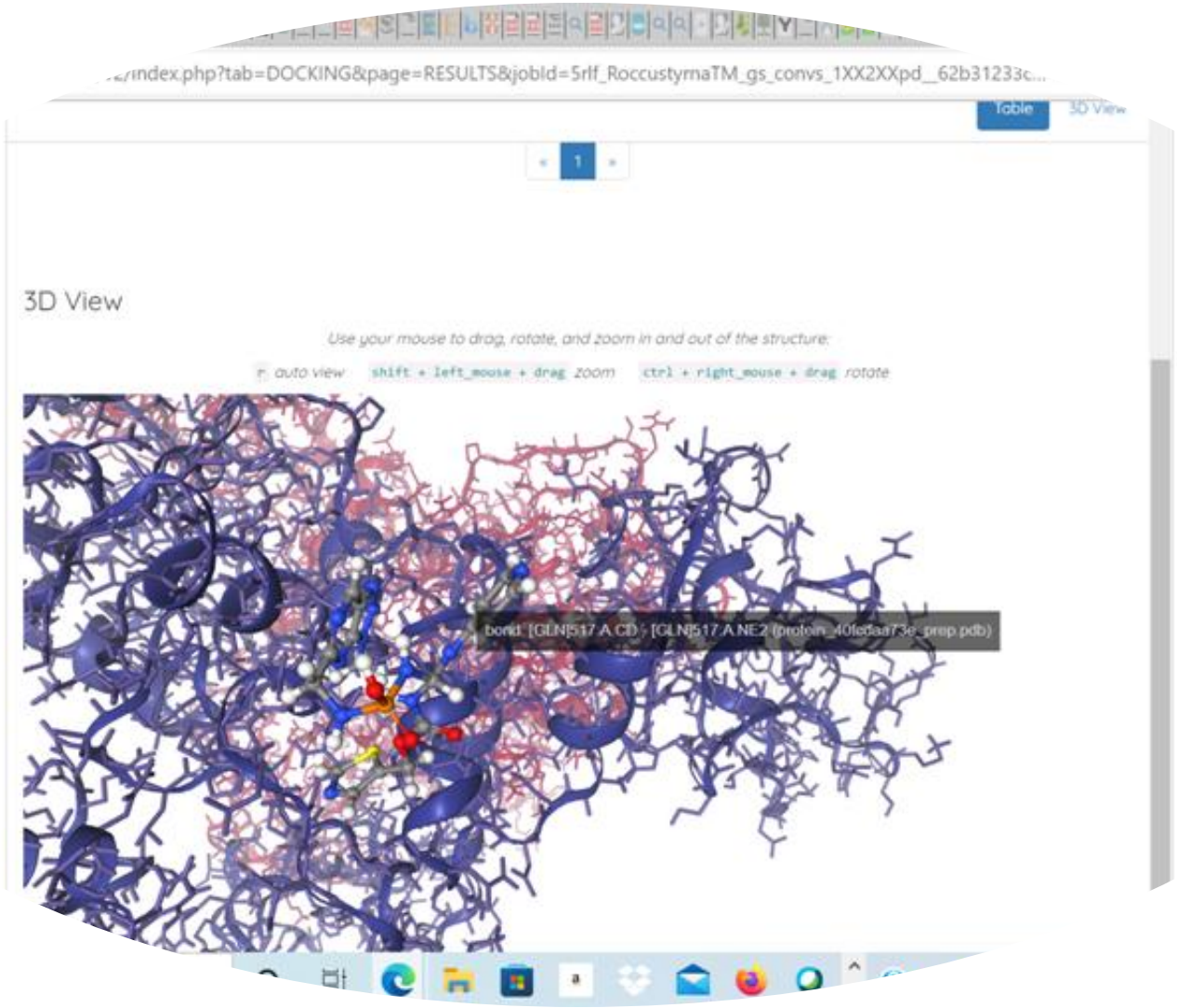
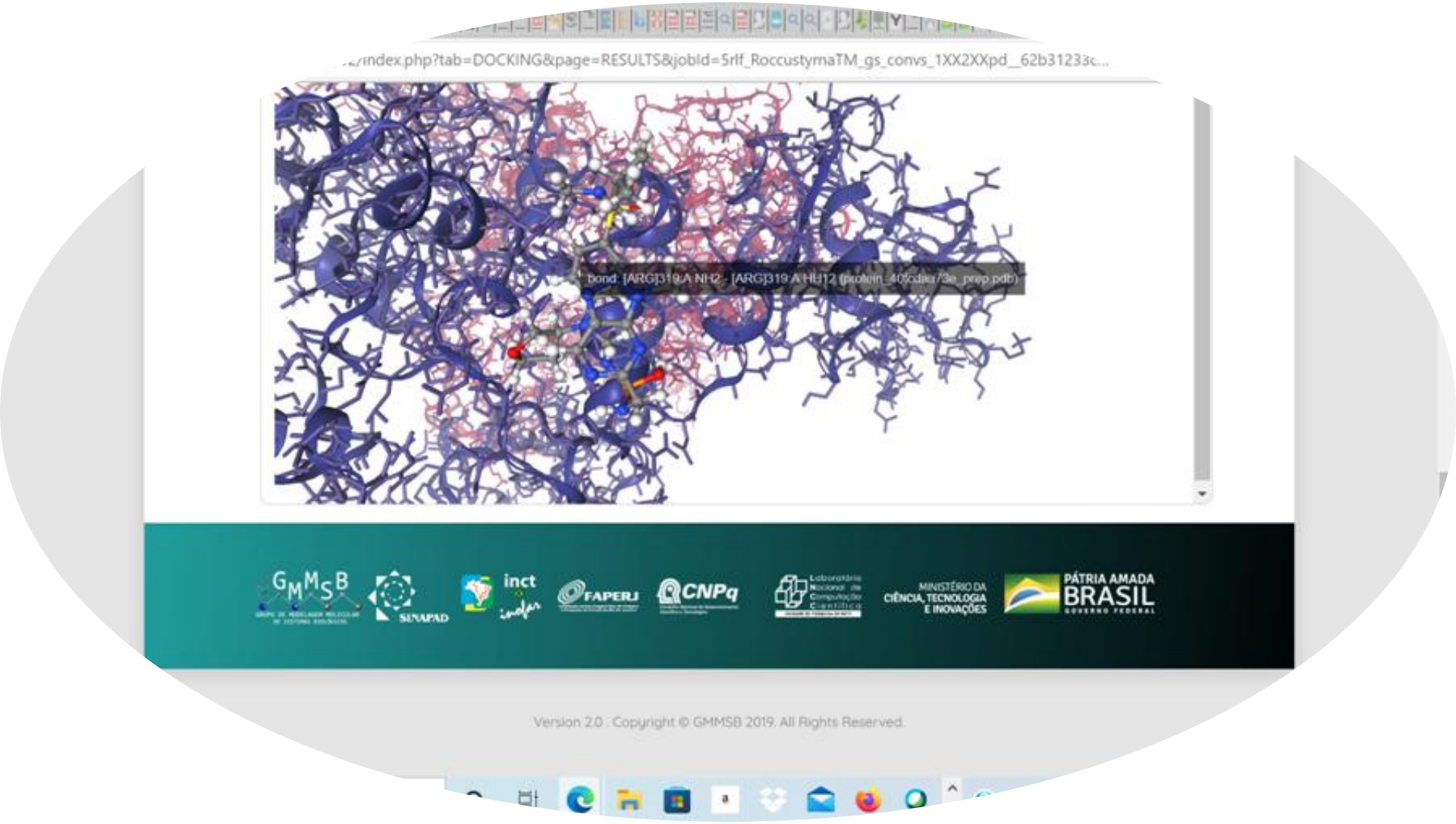
Table
3D View
Table
Rank File ID Compound Affinity Total Energy vdW Energy Elec. Energy
1 4ac5543646 ligand 1 -4.955 -101.280 -0.520 -0.159
run 2 -4.955 -101.280 -0.520 -0.159
run 9 -4.964 -101.270 -0.484 -0.188
run 2 -4.953 -101.267 -0.540 -0.130
2 54b4ef35cf ligand 1 -4.657 -26.459 -0.405 -1.310
run 10 -4.657 -26.459 -0.405 -1.310
run 7 -4.634 -26.449 -0.397 -1.292
run 10 -4.653 -26.443 -0.380 -1.320
1
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


index.php?tab=DOCKING&page=RESULTS&jobId=5rlf_RoccustyrnaTM_gs_convs_1XX2XXpd__62b31233c...
Table
3D View
1
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: [GLN]517.A.CD - [GLN]517.A.NE2 (protein_40fedaa73e_prep.pdb)


index.php?tab=DOCKING&page=RESULTS&jobId=5rlf_RoccustyrnaTM_gs_convs_1XX2XXpd__62b31233c...
bond [ARG]319:A NH2 - [ARG]319:A HH12 (protein_405daa/3e_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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