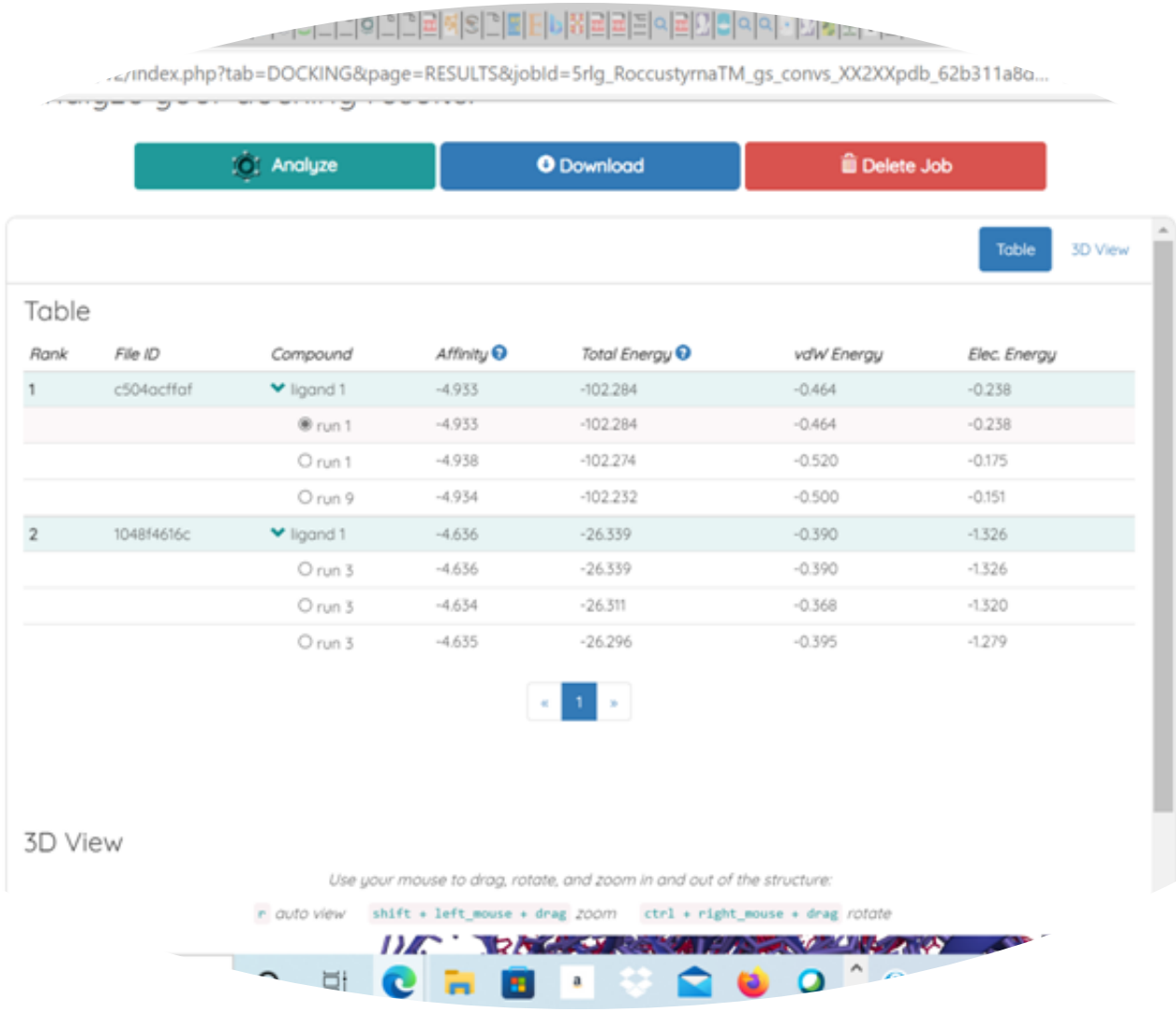
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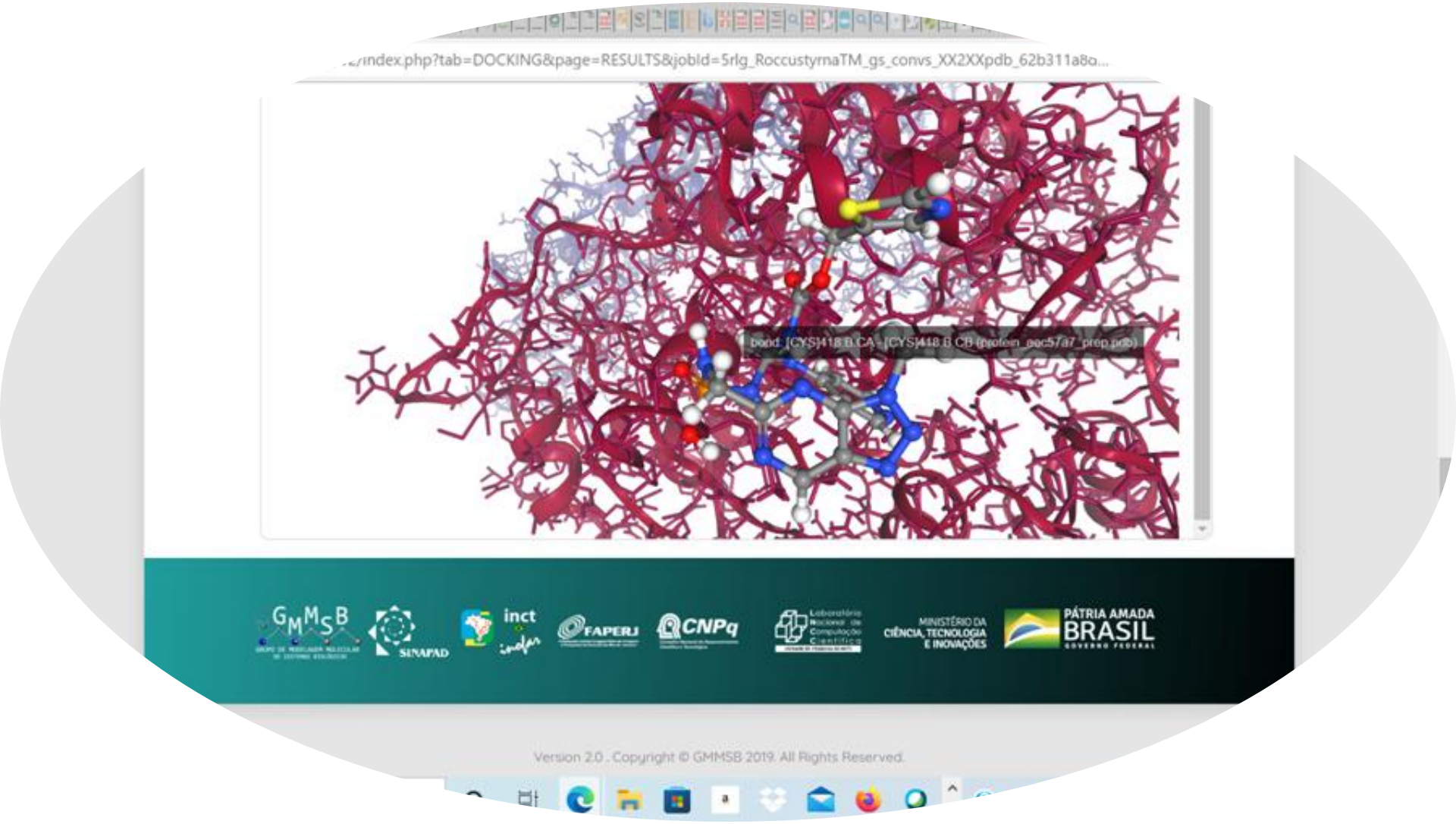
Analyze
Download
Delete Job
Table
3D View
Table
Rank
File ID
Compound
Affinity
Total Energy
vdW Energy
Elec. Energy
1
c504acffaf
ligand 1
-4.933
-102.284
-0.464
-0.238
run 1
-4.933
-102.284
-0.464
-0.238
run 1
-4.938
-102.274
-0.520
-0.175
run 9
-4.934
-102.232
-0.500
-0.151
2
1048f4616c
ligand 1
-4.636
-26.339
-0.390
-1.326
run 3
-4.636
-26.339
-0.390
-1.326
run 3
-4.634
-26.311
-0.368
-1.320
run 3
-4.635
-26.296
-0.395
-1.279
«
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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GMMSB
SINAPAD
inct
FAPERJ
CNPq
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PÁTRIA AMADA BRASIL
GOVERNO FEDERAL
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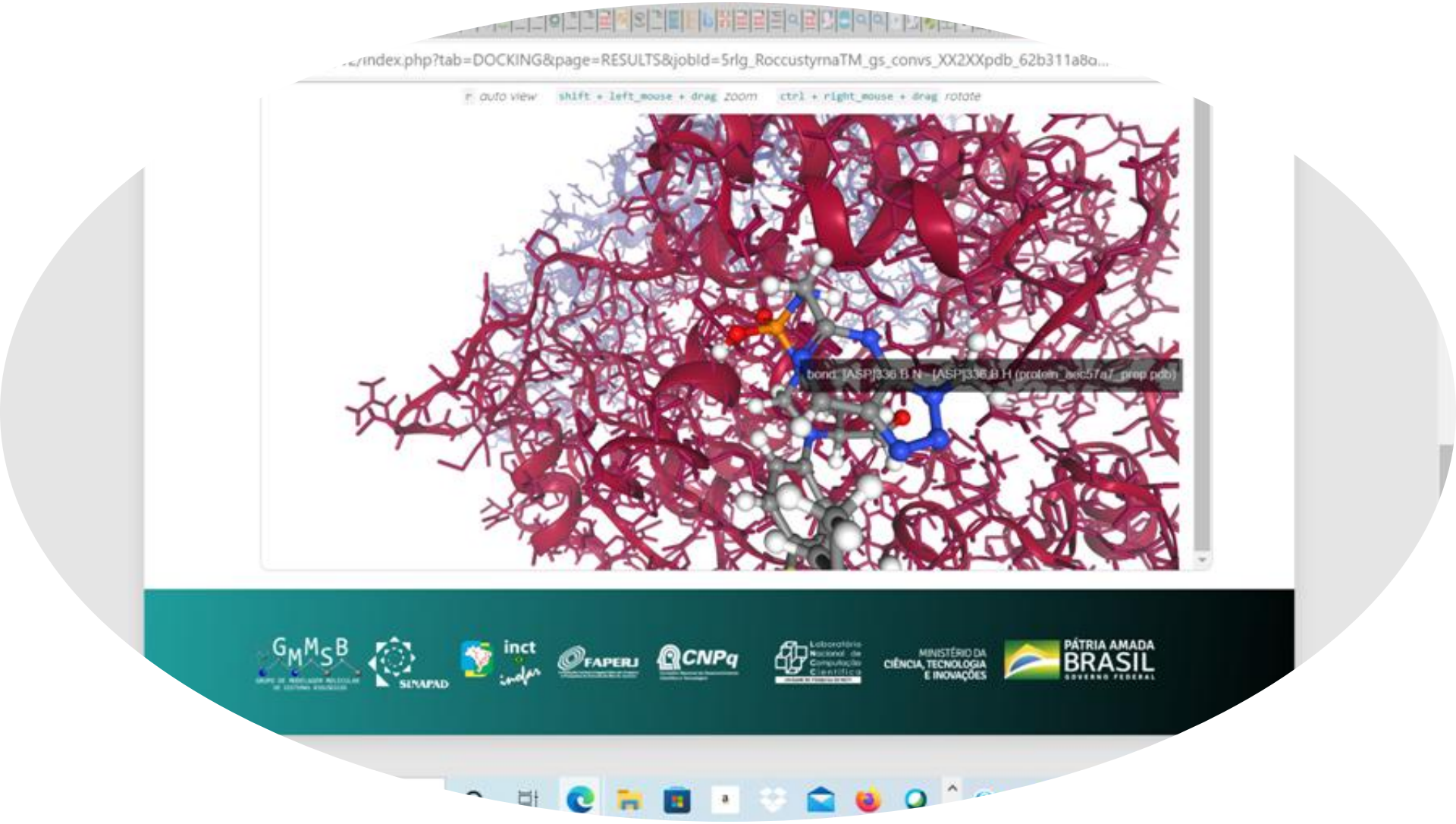
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r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [ASP]336.B.N--[ASP]336.B.H (protein_bdc57a7_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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