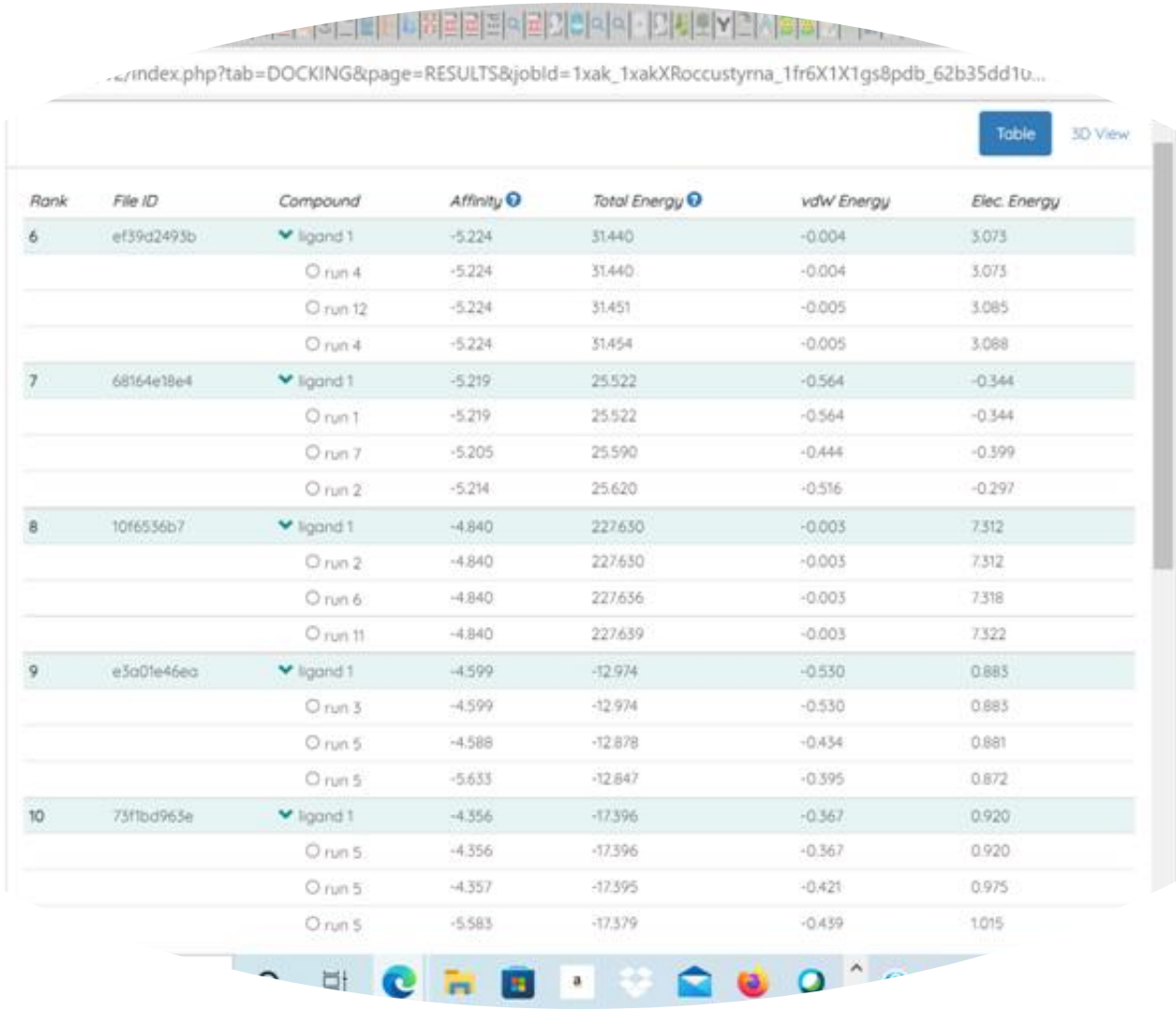
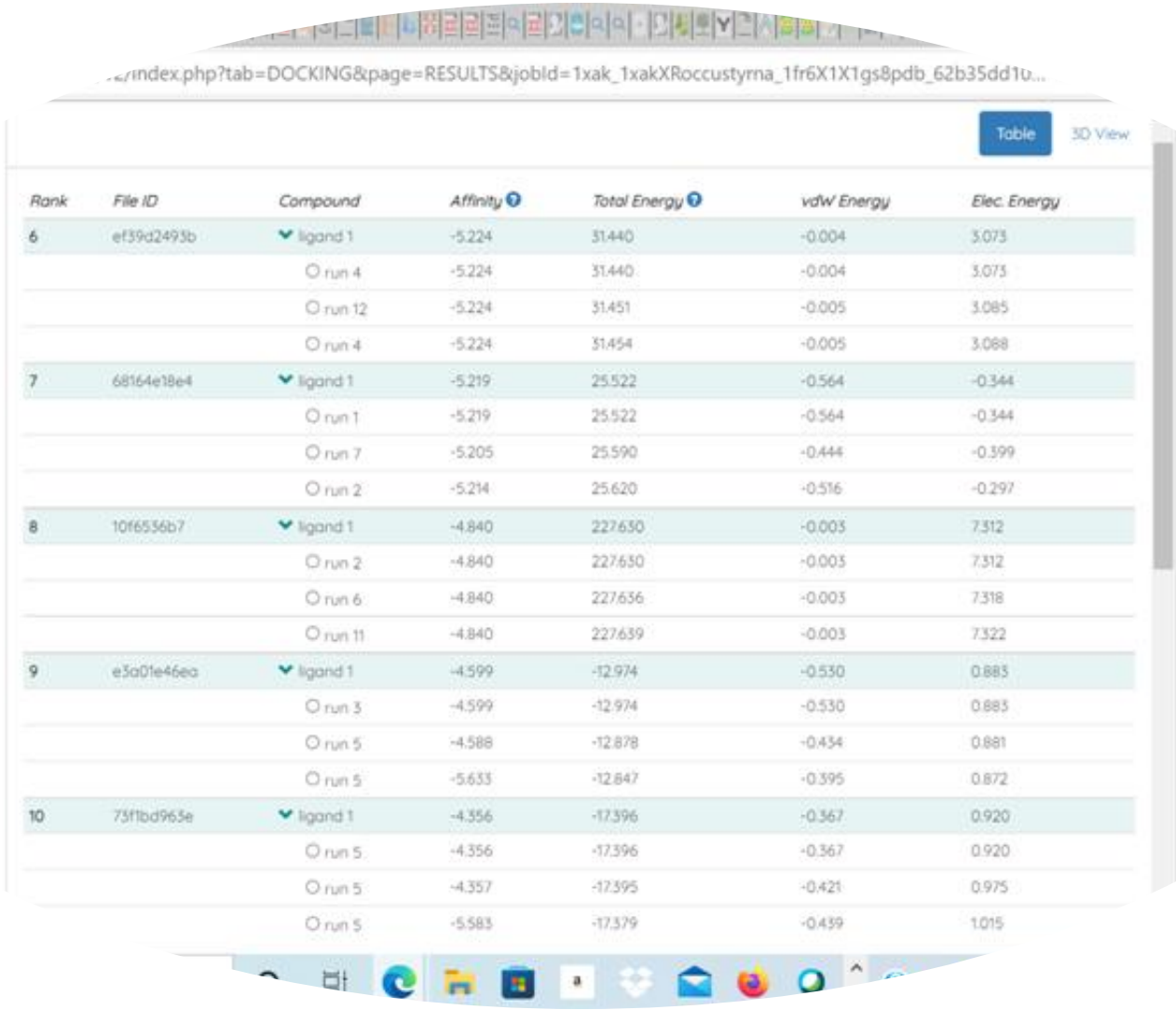


Rank	File ID	Compound	Affinity	Total Energy	vdW Energy	Elec. Energy
6	ef39d2493b	ligand 1	-5.224	31.440	-0.004	3.073
		run 4	-5.224	31.440	-0.004	3.073
		run 12	-5.224	31.451	-0.005	3.085
		run 4	-5.224	31.454	-0.005	3.088
7	68164e18e4	ligand 1	-5.219	25.522	-0.564	-0.344
		run 1	-5.219	25.522	-0.564	-0.344
		run 7	-5.205	25.590	-0.444	-0.399
		run 2	-5.214	25.620	-0.516	-0.297
8	10f6556b7	ligand 1	-4.840	227.630	-0.003	7.312
		run 2	-4.840	227.630	-0.003	7.312
		run 6	-4.840	227.636	-0.003	7.318
		run 11	-4.840	227.639	-0.003	7.322
9	e3a01e46ea	ligand 1	-4.599	-12.974	-0.530	0.883
		run 3	-4.599	-12.974	-0.530	0.883
		run 5	-4.588	-12.878	-0.434	0.881
		run 5	-5.633	-12.847	-0.395	0.872
10	73f1bd965e	ligand 1	-4.356	-17.396	-0.367	0.920
		run 5	-4.356	-17.396	-0.367	0.920
		run 5	-4.357	-17.395	-0.421	0.975
		run 5	-5.583	-17.379	-0.439	1.015



Rank	File ID	Compound	Affinity	Total Energy	vdW Energy	Elec. Energy
6	ef39d2493b	ligand 1	-5.224	31.440	-0.004	3.073
		run 4	-5.224	31.440	-0.004	3.073
		run 12	-5.224	31.451	-0.005	3.085
		run 4	-5.224	31.454	-0.005	3.088
7	68164e18e4	ligand 1	-5.219	25.522	-0.564	-0.344
		run 1	-5.219	25.522	-0.564	-0.344
		run 7	-5.205	25.590	-0.444	-0.399
		run 2	-5.214	25.620	-0.516	-0.297
8	10f6556b7	ligand 1	-4.840	227.630	-0.003	7.312
		run 2	-4.840	227.630	-0.003	7.312
		run 6	-4.840	227.636	-0.003	7.318
		run 11	-4.840	227.639	-0.003	7.322
9	e3a01e46ea	ligand 1	-4.599	-12.974	-0.530	0.883
		run 3	-4.599	-12.974	-0.530	0.883
		run 5	-4.588	-12.878	-0.434	0.881
		run 5	-5.633	-12.847	-0.395	0.872
10	73f1bd965e	ligand 1	-4.356	-17.396	-0.367	0.920
		run 5	-4.356	-17.396	-0.367	0.920
		run 5	-4.357	-17.395	-0.421	0.975
		run 5	-5.583	-17.379	-0.439	1.015

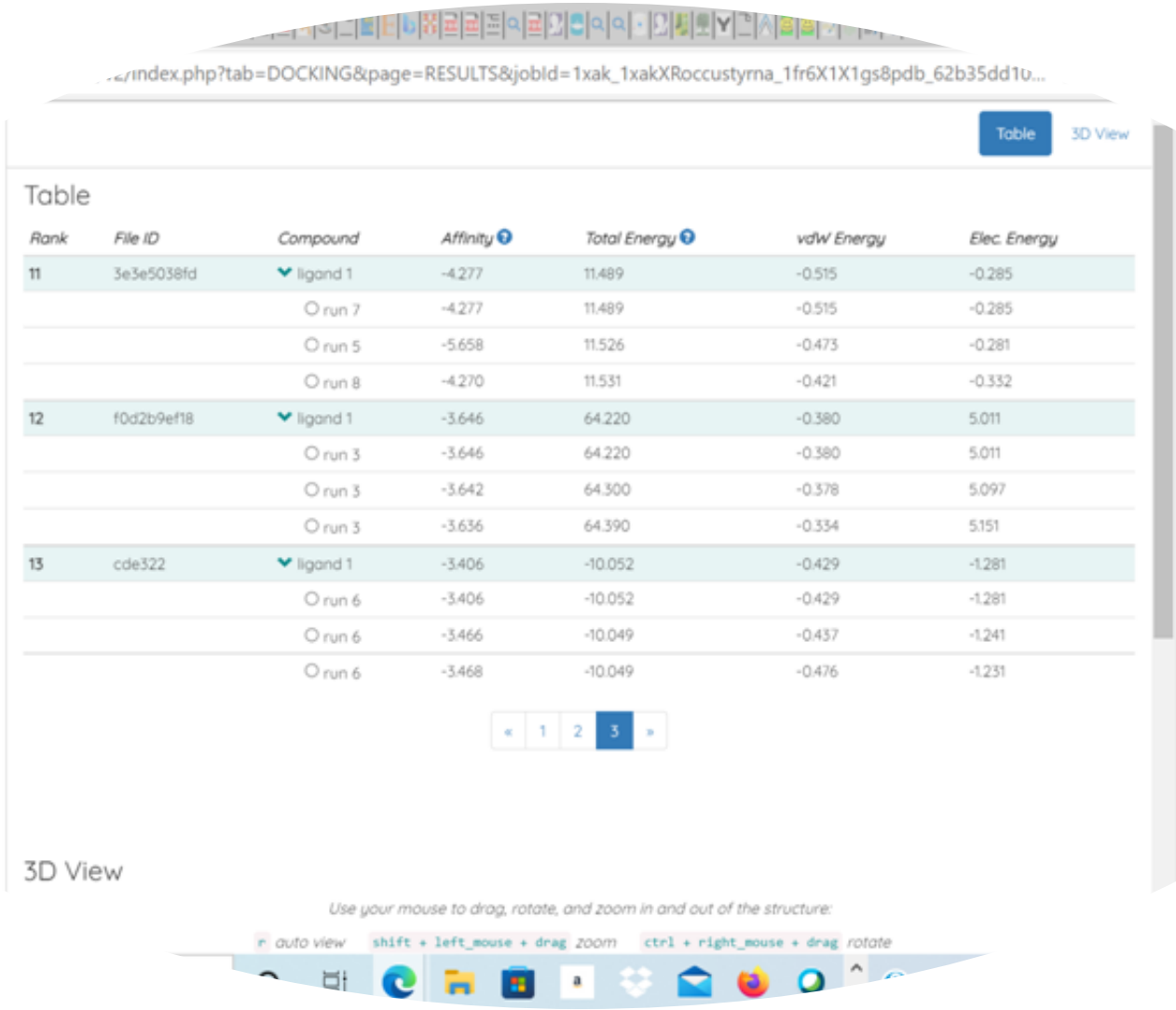

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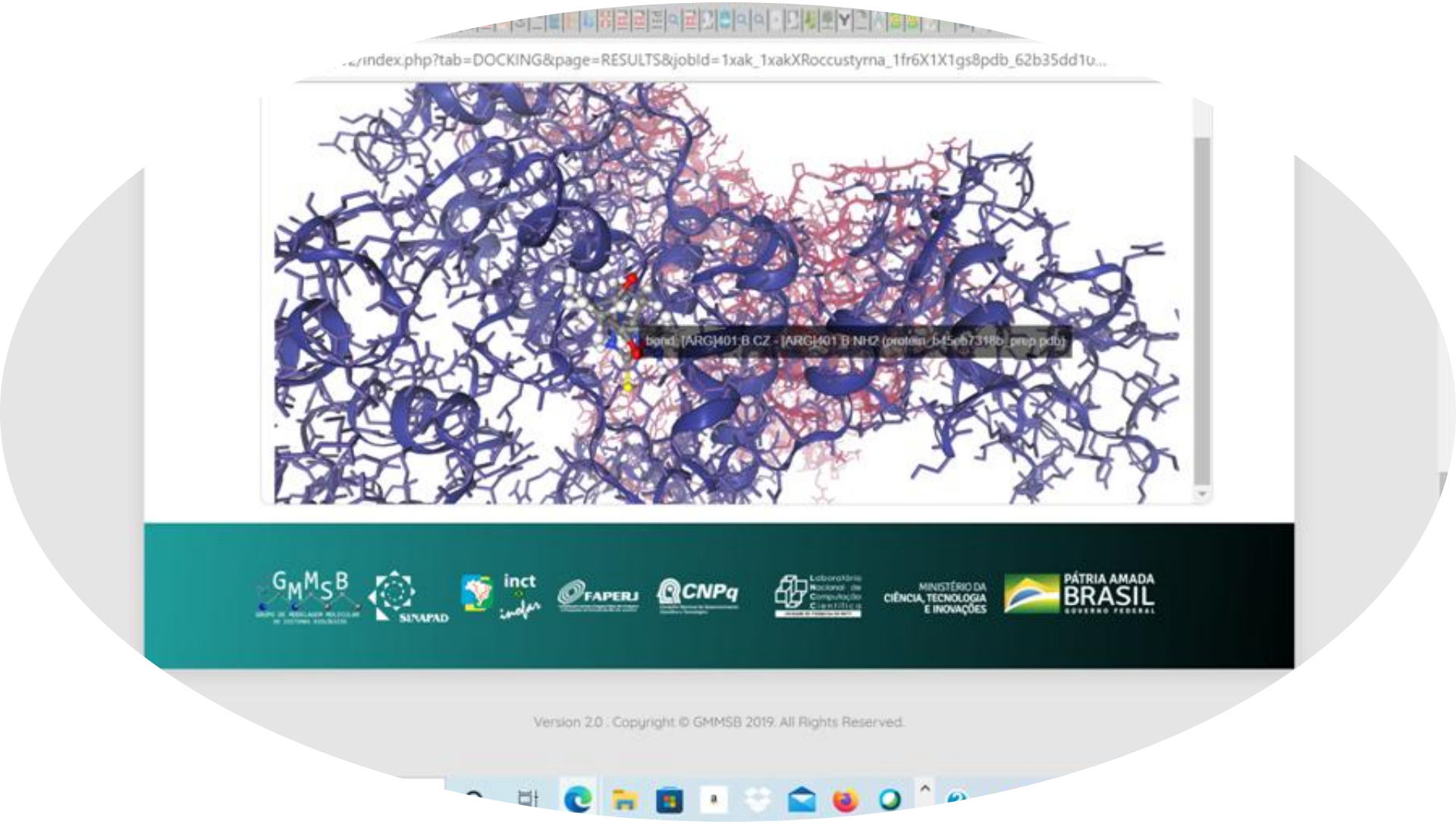
Table
3D View
Table
Rank File ID Compound Affinity Total Energy vdW Energy Elec. Energy
11 3e3e5038fd ligand 1 -4.277 11.489 -0.515 -0.285
run 7 -4.277 11.489 -0.515 -0.285
run 5 -5.658 11.526 -0.473 -0.281
run 8 -4.270 11.531 -0.421 -0.332
12 f0d2b9ef18 ligand 1 -3.646 64.220 -0.380 5.011
run 3 -3.646 64.220 -0.380 5.011
run 3 -3.642 64.300 -0.378 5.097
run 3 -3.636 64.390 -0.334 5.151
13 cde322 ligand 1 -3.406 -10.052 -0.429 -1.281
run 6 -3.406 -10.052 -0.429 -1.281
run 6 -3.466 -10.049 -0.437 -1.241
run 6 -3.468 -10.049 -0.476 -1.231
« 1 2 3 »
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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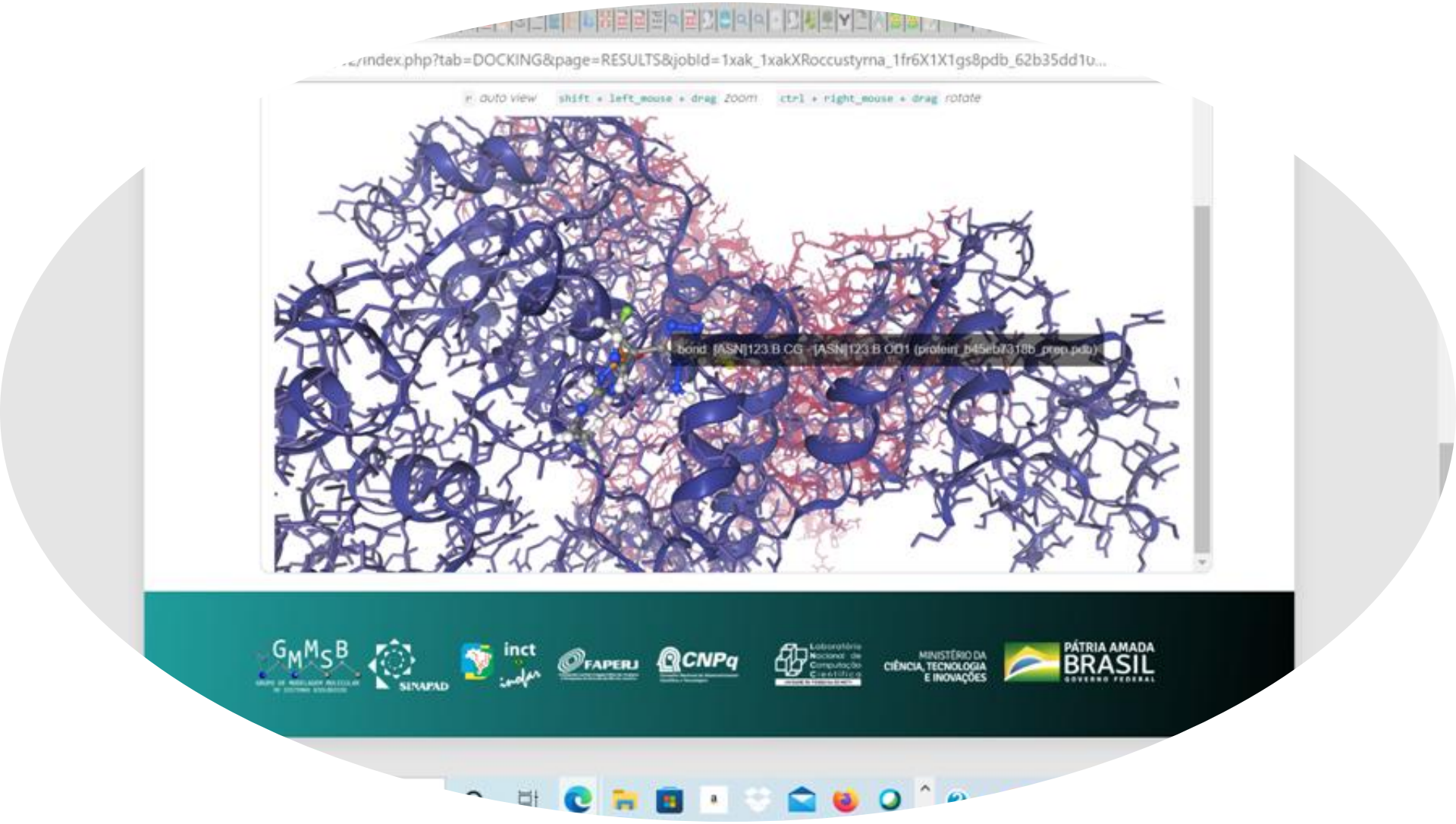
index.php?tab=DOCKING&page=RESULTS&jobId=1xak_1xakXRoccustyrna_1fr6X1X1gs8pdb_62b35dd1u...
r: auto view
shift + left_mouse + drag: zoom
ctrl + right_mouse + drag: rotate
bond: [ASN]123:B:CG - [ASN]123:B:OD1 (protein_b45eb7318b_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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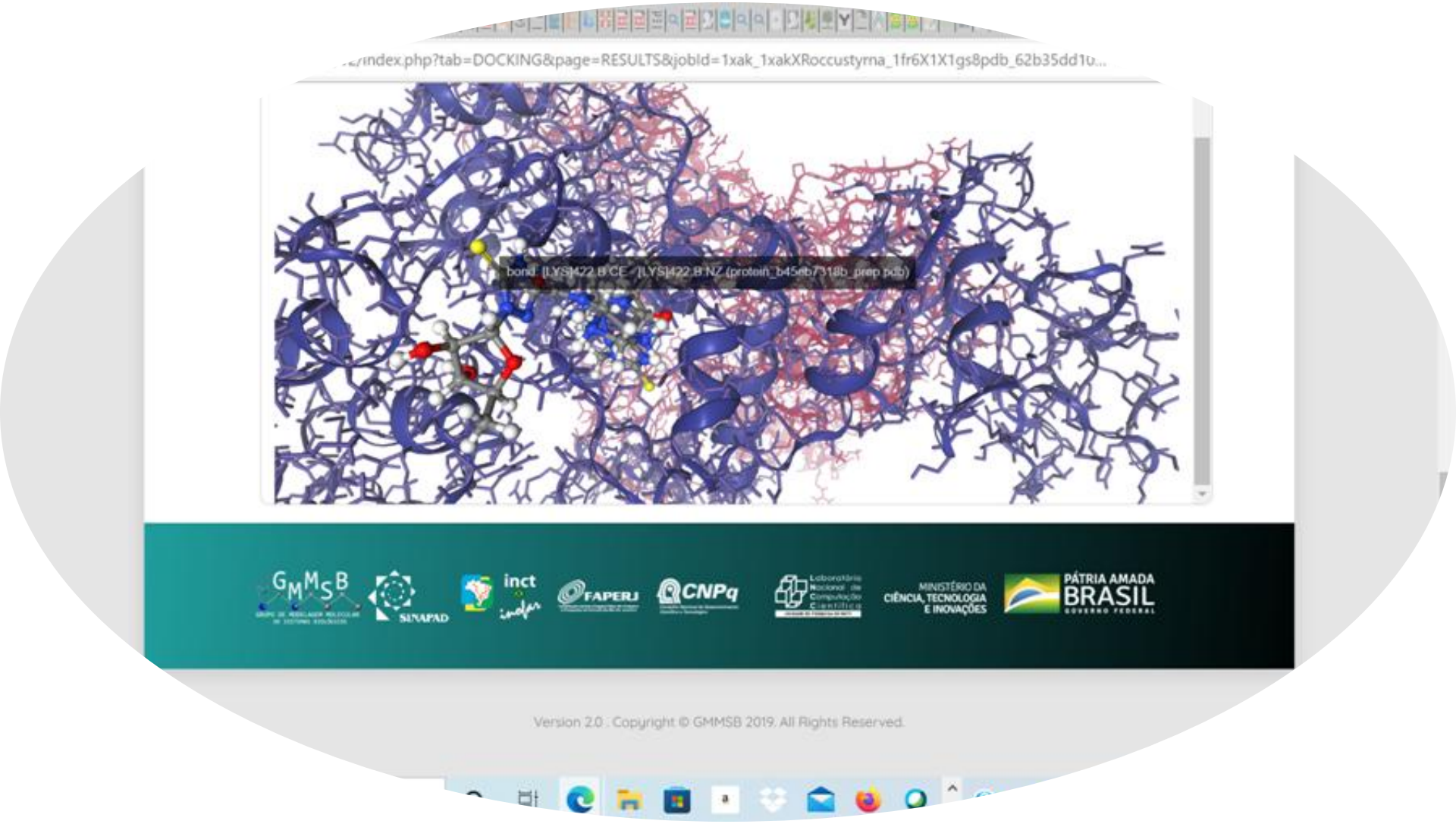
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bond: [LYS]422.B.CE - [LYS]422.B.NZ (protein_b45eb7318b_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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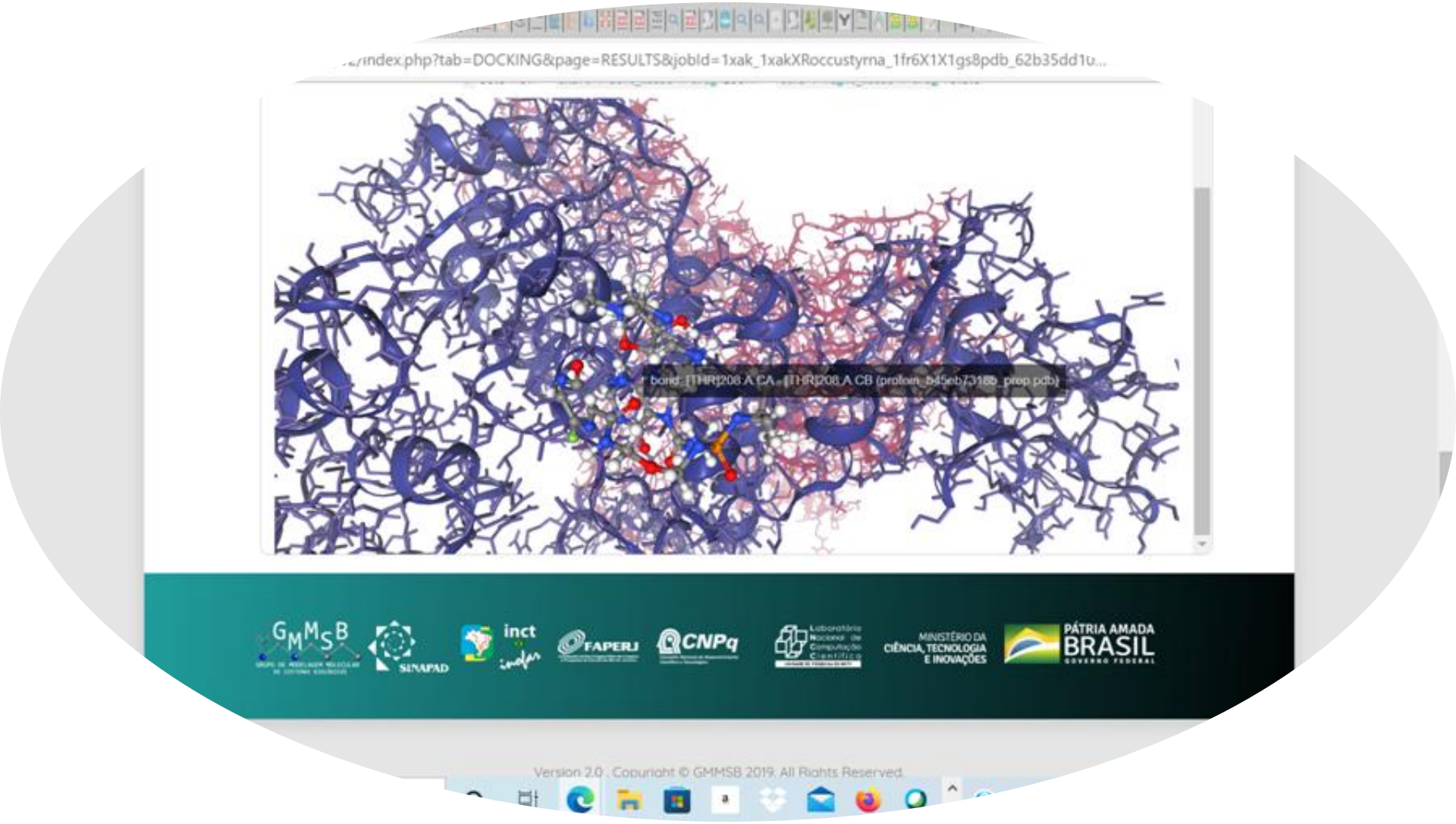
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bond: [THR]208:A:CA - [THR]208:A:CB (protein_b45eb7318b_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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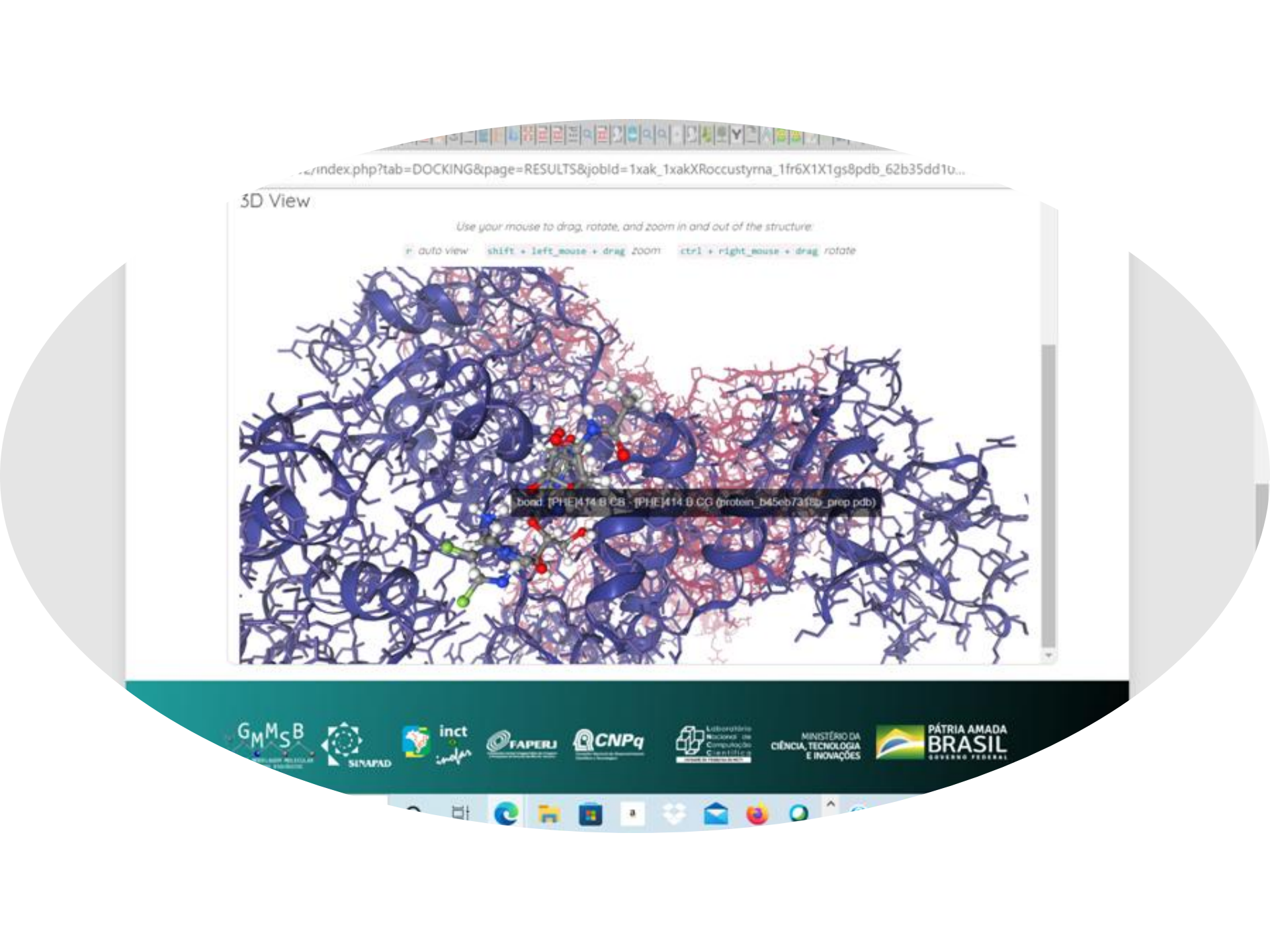
index.php?tab=DOCKING&page=RESULTS&jobId=1xak_1xakXRoccustyrna_1fr6X1X1gs8pdb_62b35dd1u...
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [PHE]414:B:CB - [PHE]414:B:CG (protein_b45eb73f8b_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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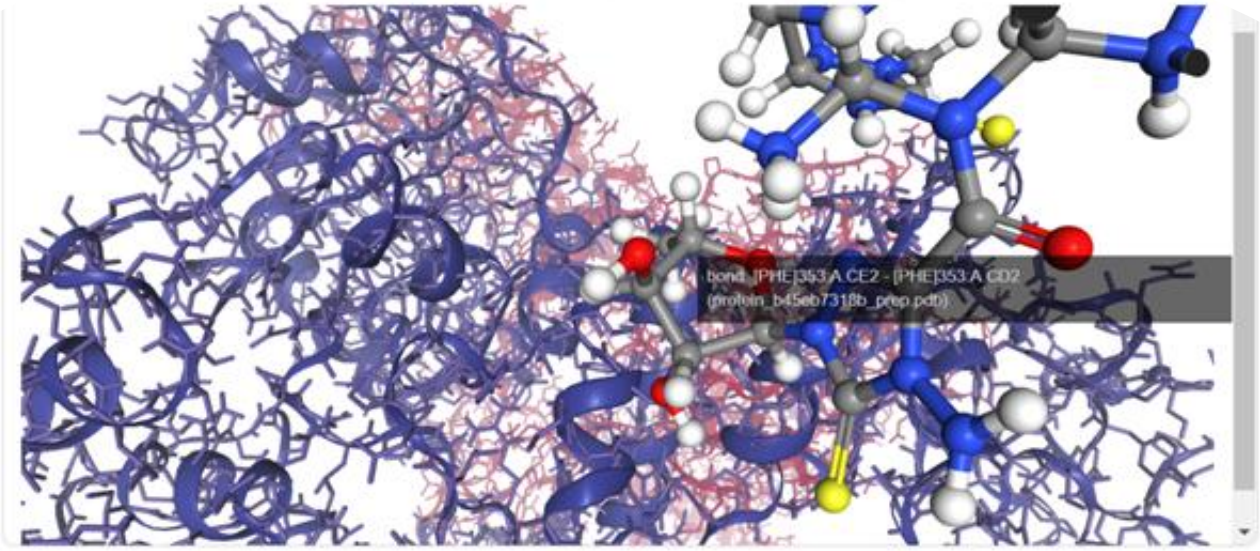

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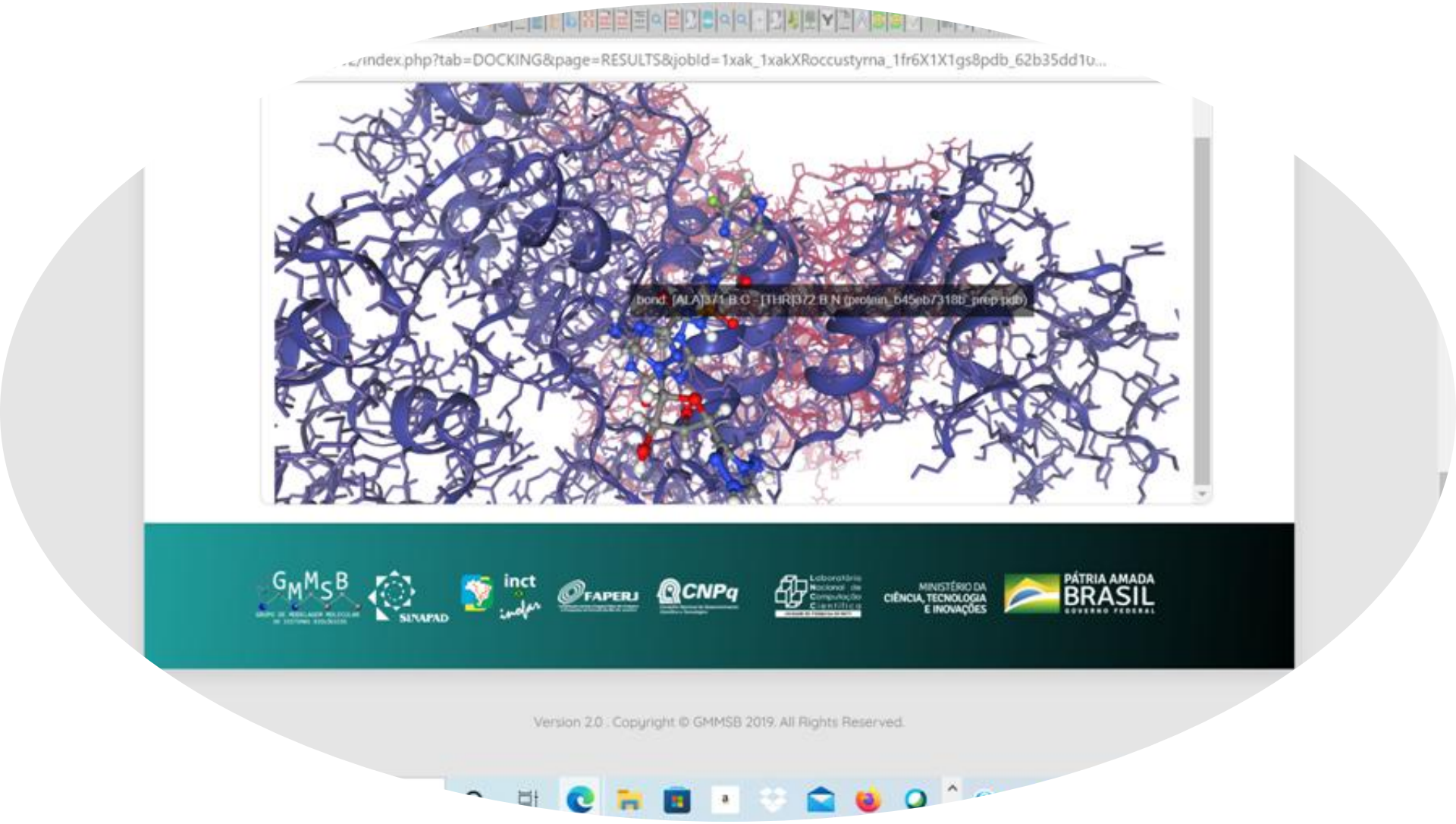
index.php?tab=DOCKING&page=RESULTS&jobId=1xak_1xakXRoccustyrna_1fr6X1X1gs8pdb_62b35dd1u...
bond: [ALA]371.B.C - [THR]372.B.N (protein_645eb7318b_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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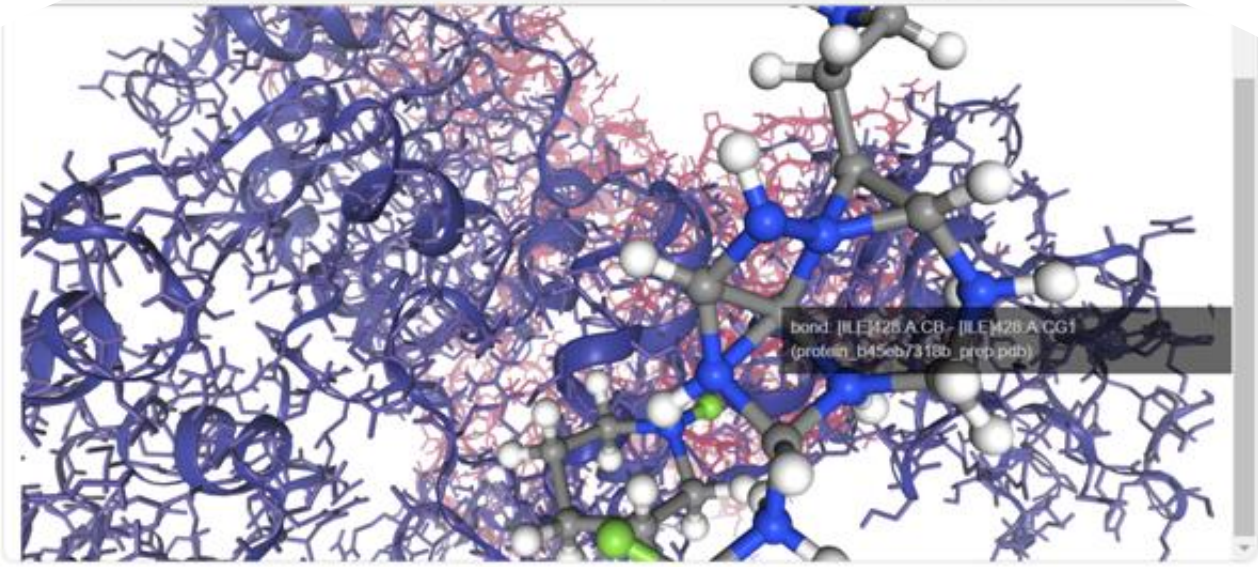

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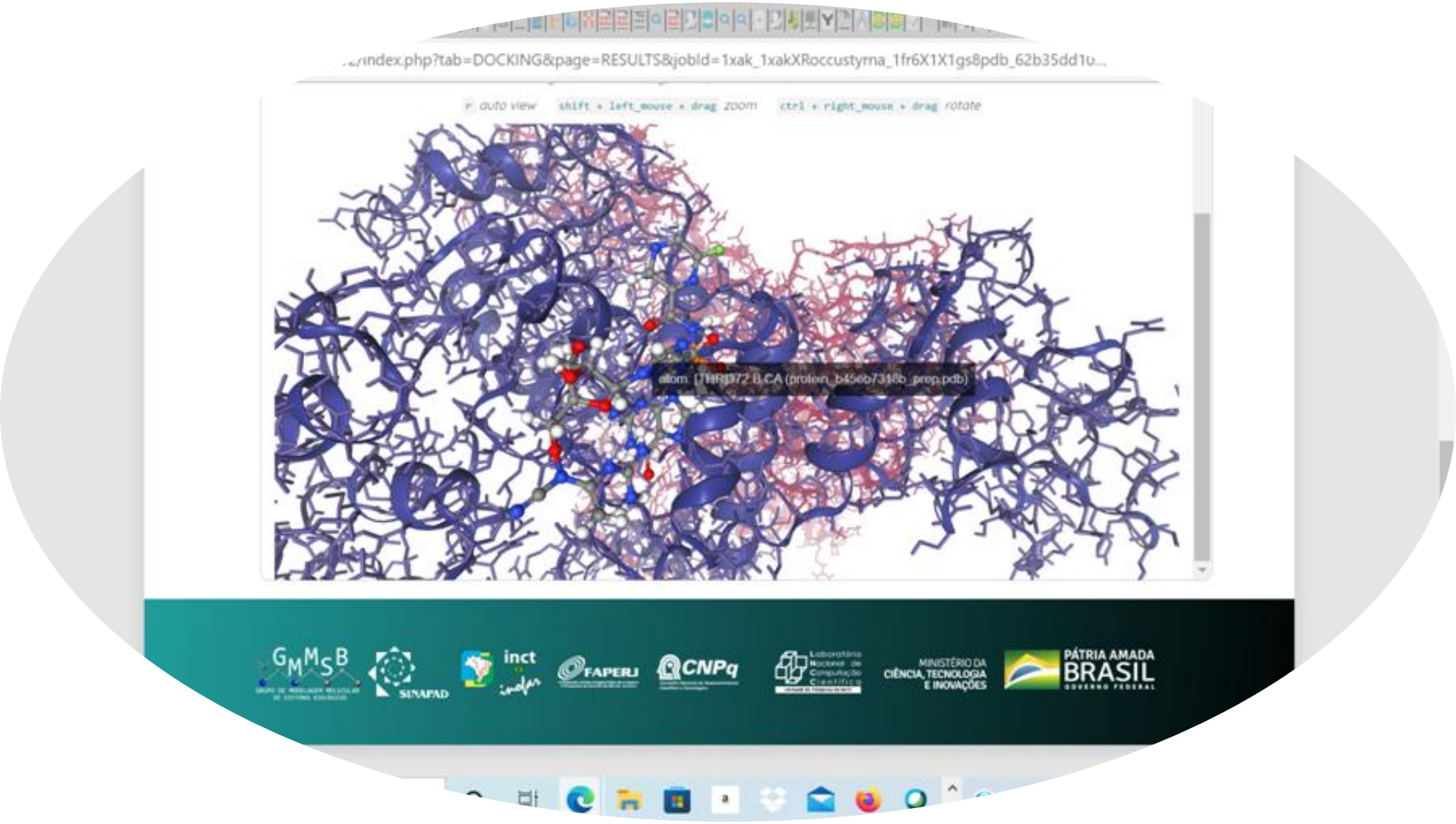
index.php?tab=DOCKING&page=RESULTS&jobId=1xak_1xakXRoccustyrna_1fr6X1X1gs8pdb_62b35dd1u...
auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
atom: [THR]372:B.CA (protein_b45eb7318b_prep.pdb)
GMMSB
SINAPAD
inct
inofar
FAPERJ
CNPq
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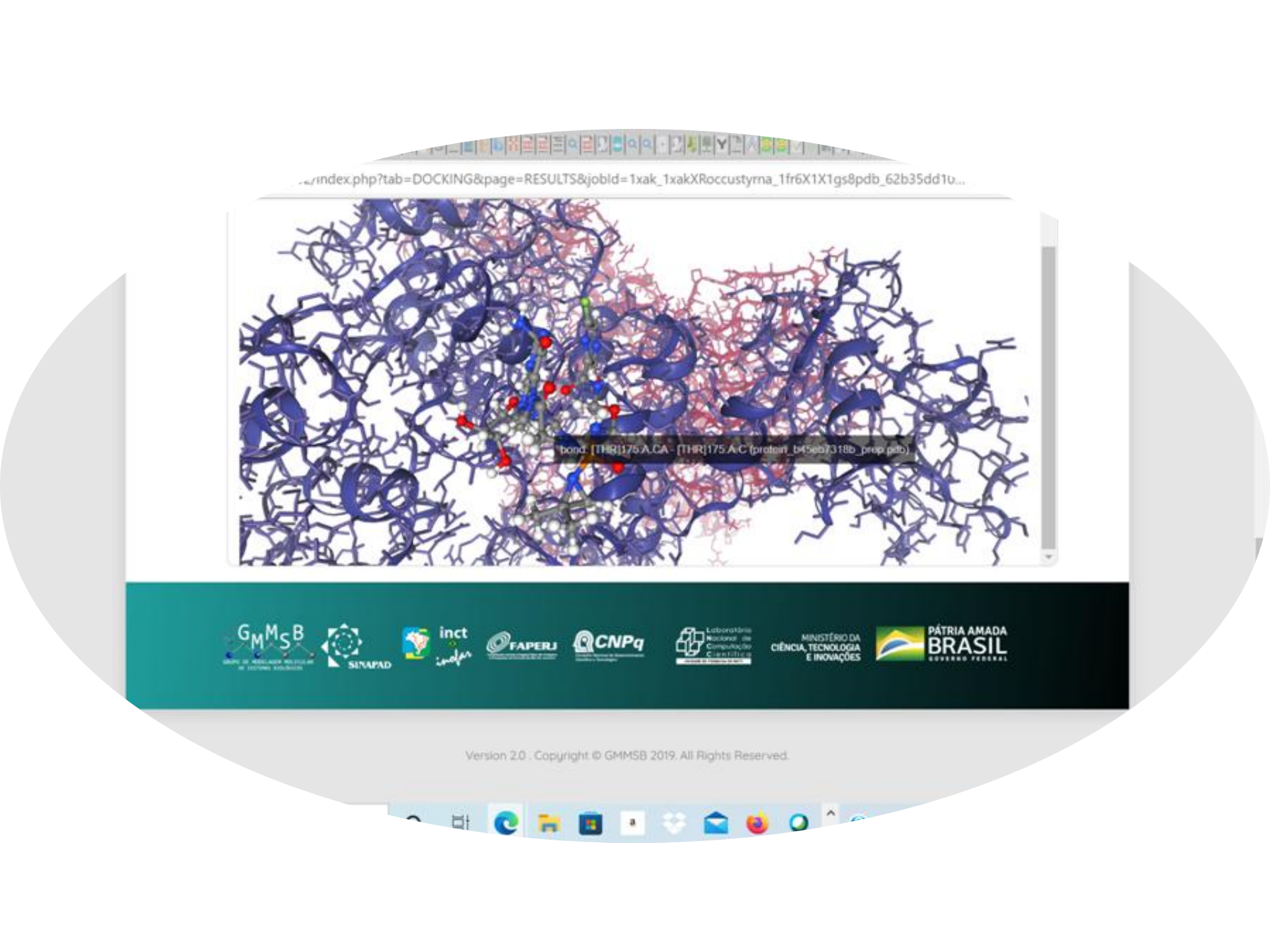
index.php?tab=DOCKING&page=RESULTS&jobId=1xak_1xakXRoccustyrna_1fr6X1X1gs8pdb_62b35dd1u...
bond: [THR]175:A:CA - [THR]175:A:C (protein_b45eb7318b_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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index.php?tab=DOCKING&page=RESULTS&jobId=1xak_1xakXRoccustyrna_1fr6X1X1gs8pdb_62b35dd1u...

Table | 3D View

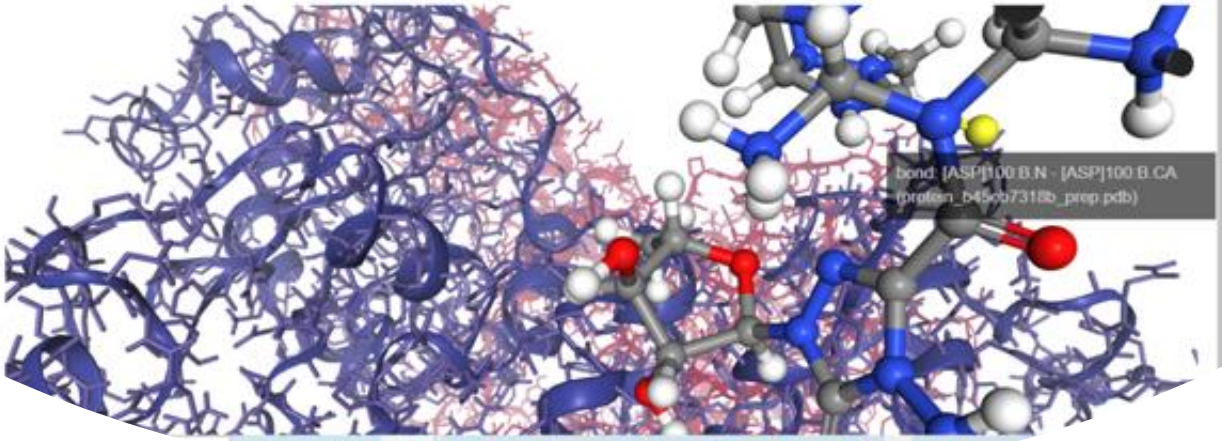
O run 5	-4.356	-17.396	-0.367	0.920
O run 5	-4.357	-17.395	-0.421	0.975
O run 5	-5.583	-17.379	-0.439	1.015

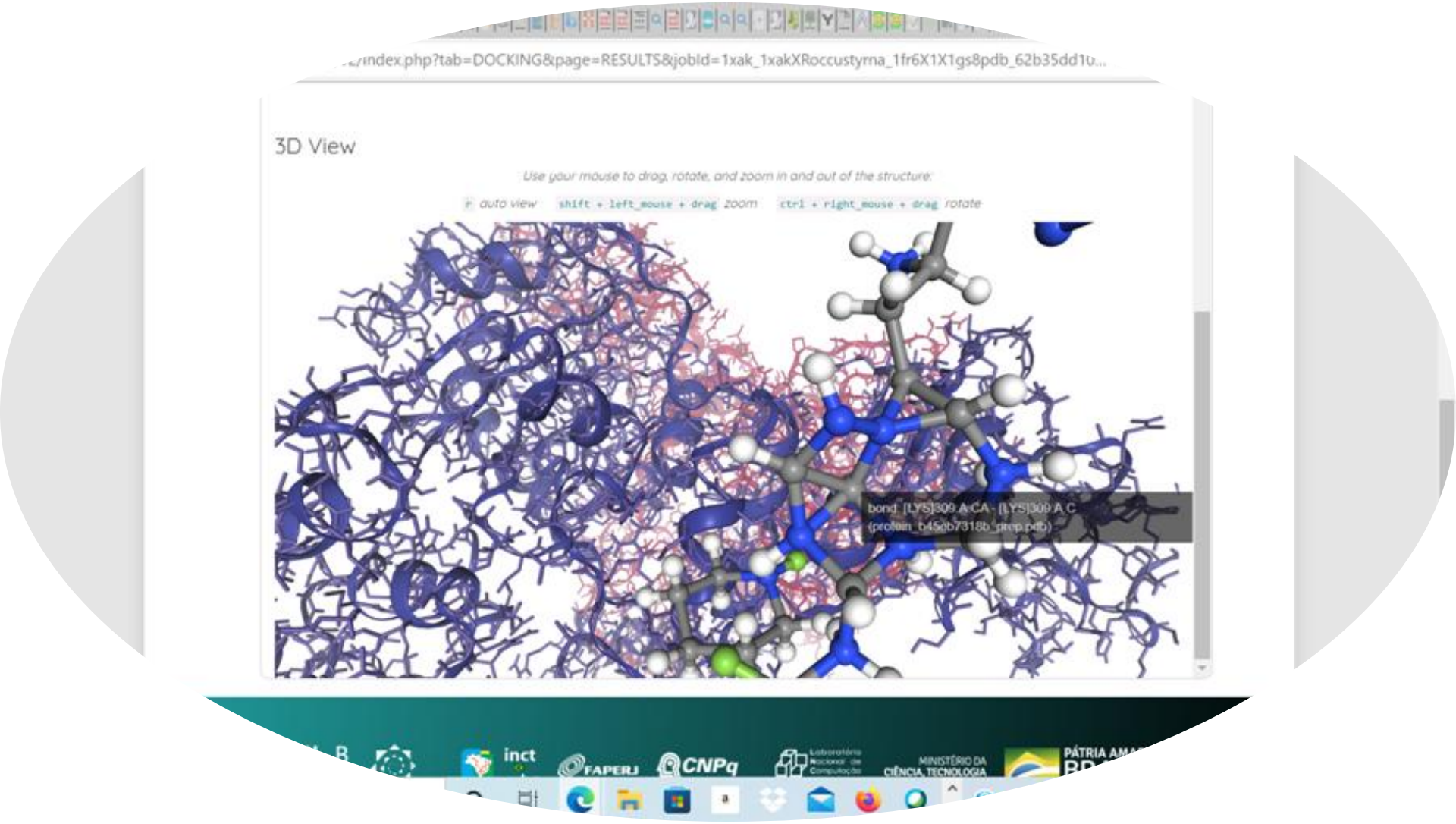
« 1 2 3 »

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=1xak_1xakXRoccustyrna_1fr6X1X1gs8pdb_62b35dd1u...
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 [LYS]309 A:CA - [LYS]309 A:C
(protein_b45db7318b_prep.pdb)
inct
FAPERJ
CNPq
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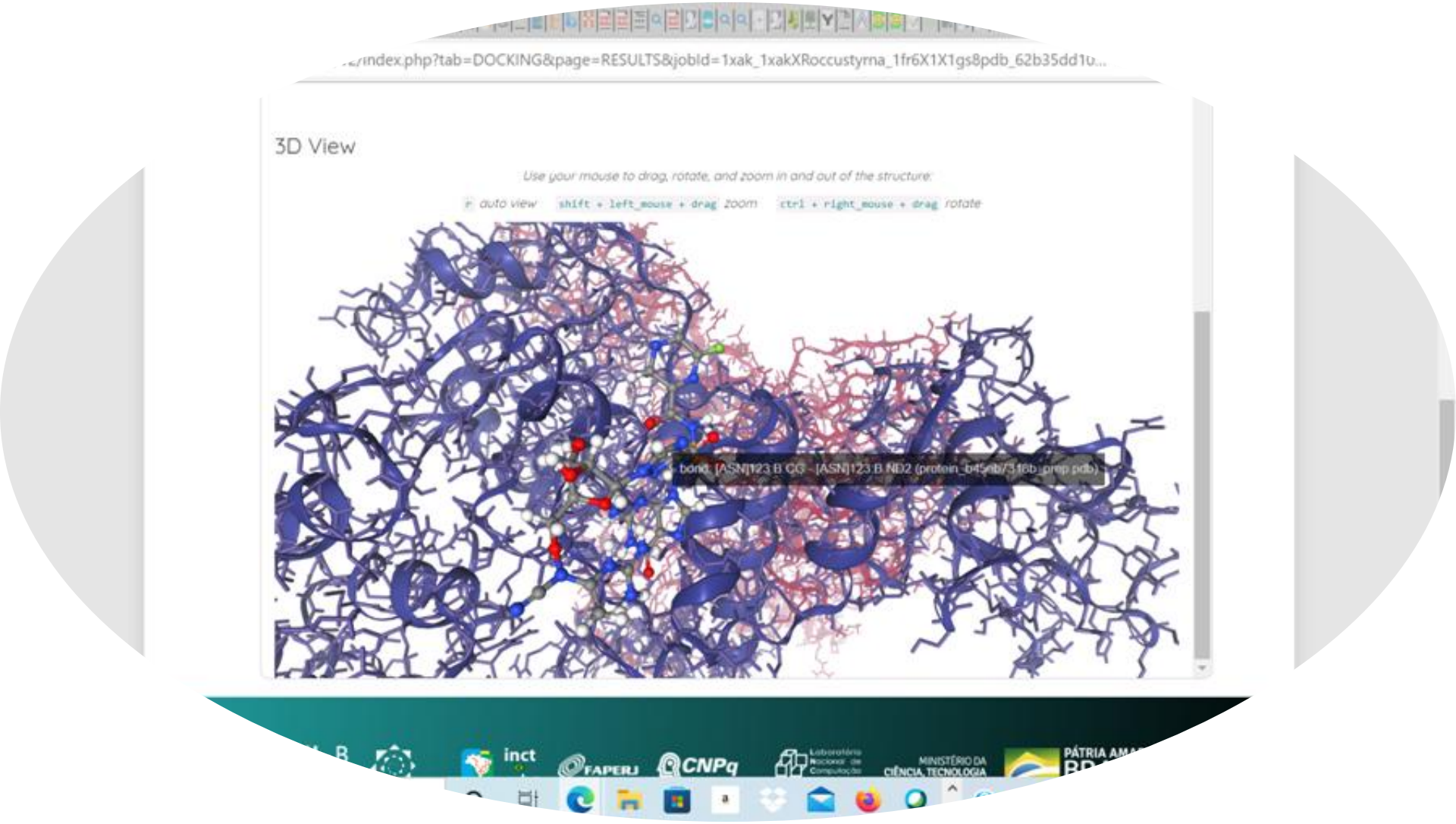
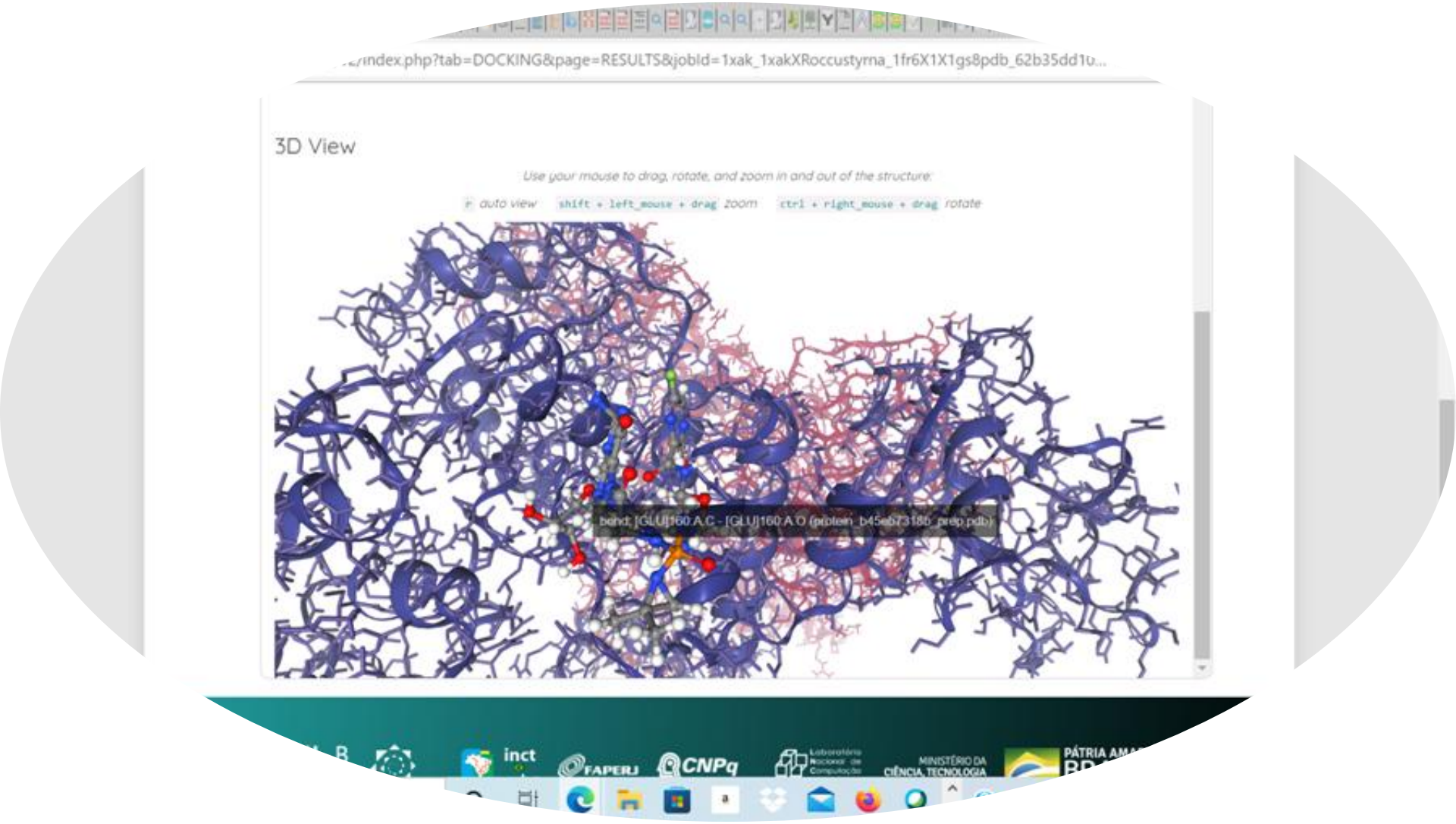

index.php?tab=DOCKING&page=RESULTS&jobId=1xak_1xakXRoccustyrna_1fr6X1X1gs8pdb_62b35dd1u...
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure:
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [ASN]123.B.CG - [ASN]123.B.ND2 (protein_b45nb/3.16b_prep.pdb)
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA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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: [GLU]160:A.C - [GLU]160:A.O (protein_b45eb73180_prep.pdb)
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA

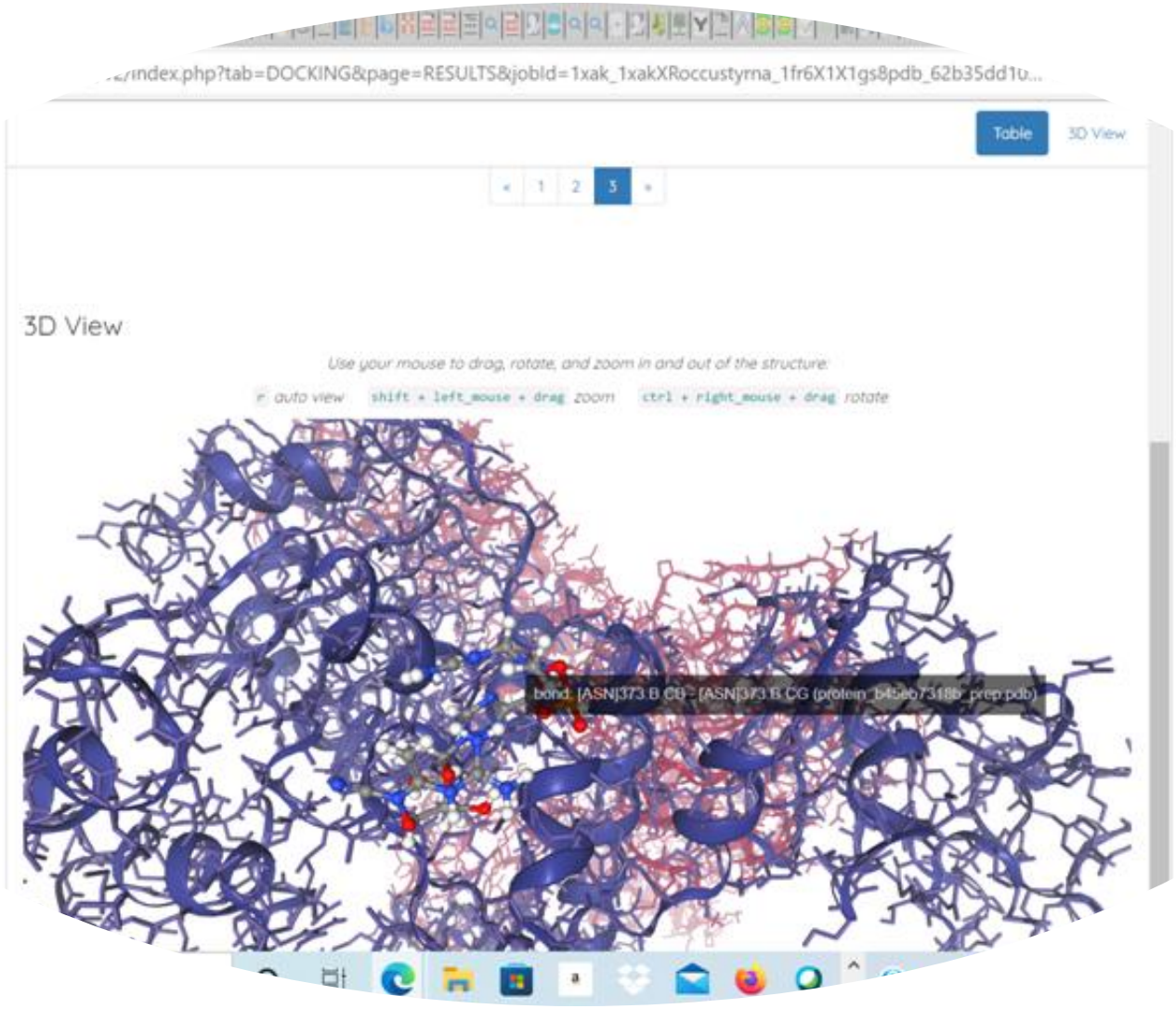
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Table
3D View
« 1 2 3 »
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [ASN]373.B.CB - [ASN]373.B.CG (protein_b45bb7318b_prep.pdb)

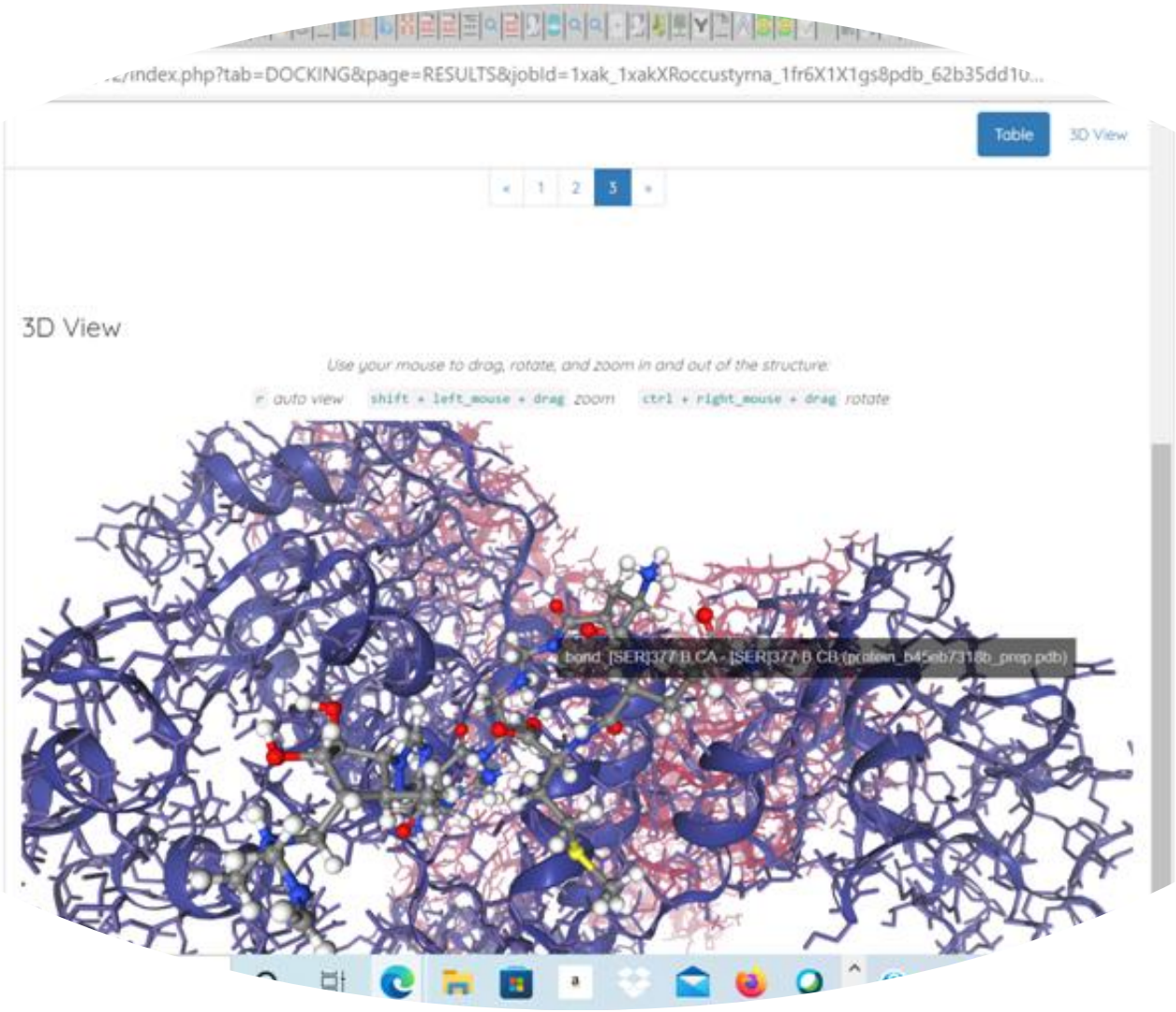
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Table
3D View
« 1 2 3 »
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond [SER]377:B.CA - [SER]377:B.CB (protein_b45eb7318b_prep.pdb)

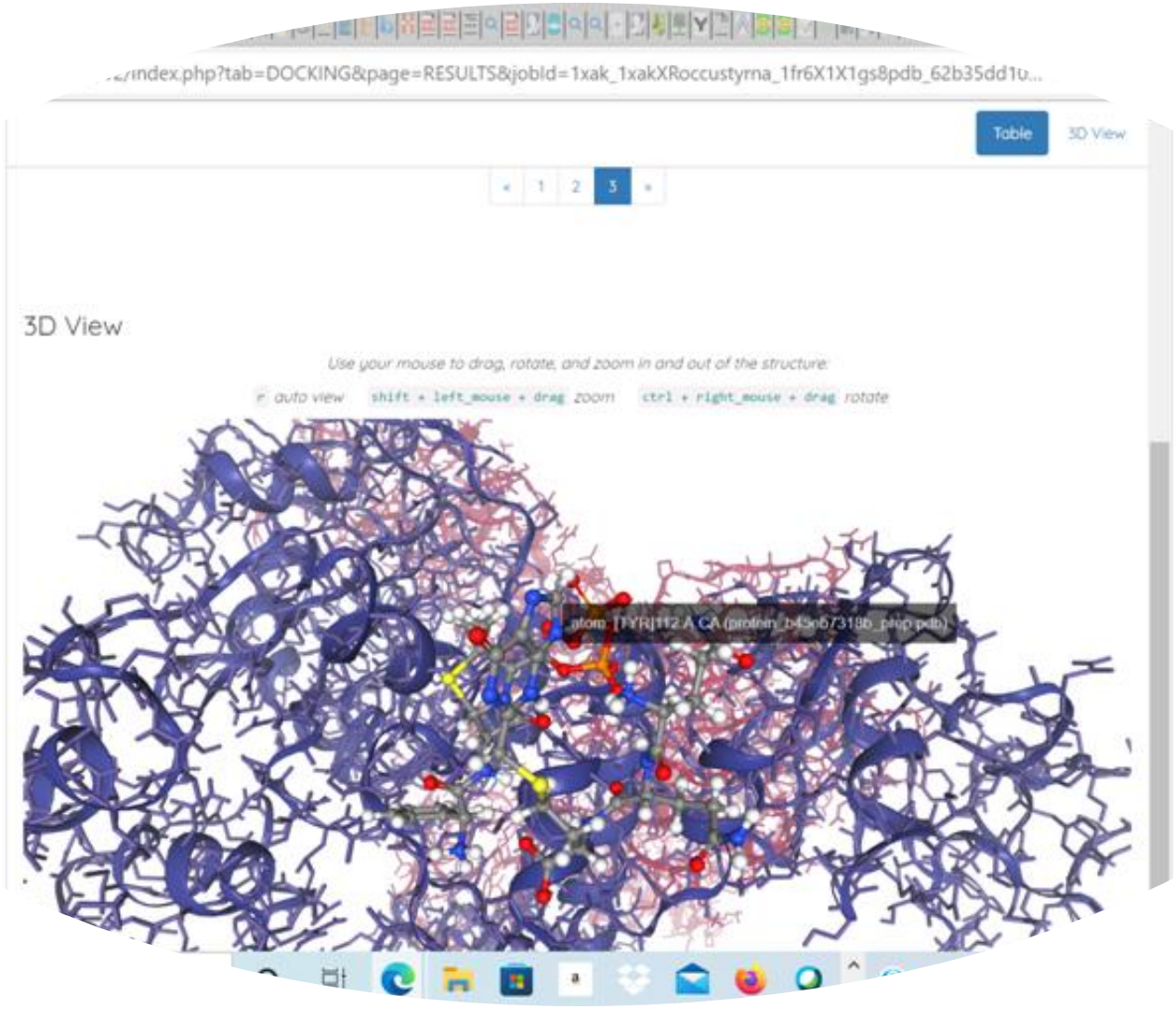
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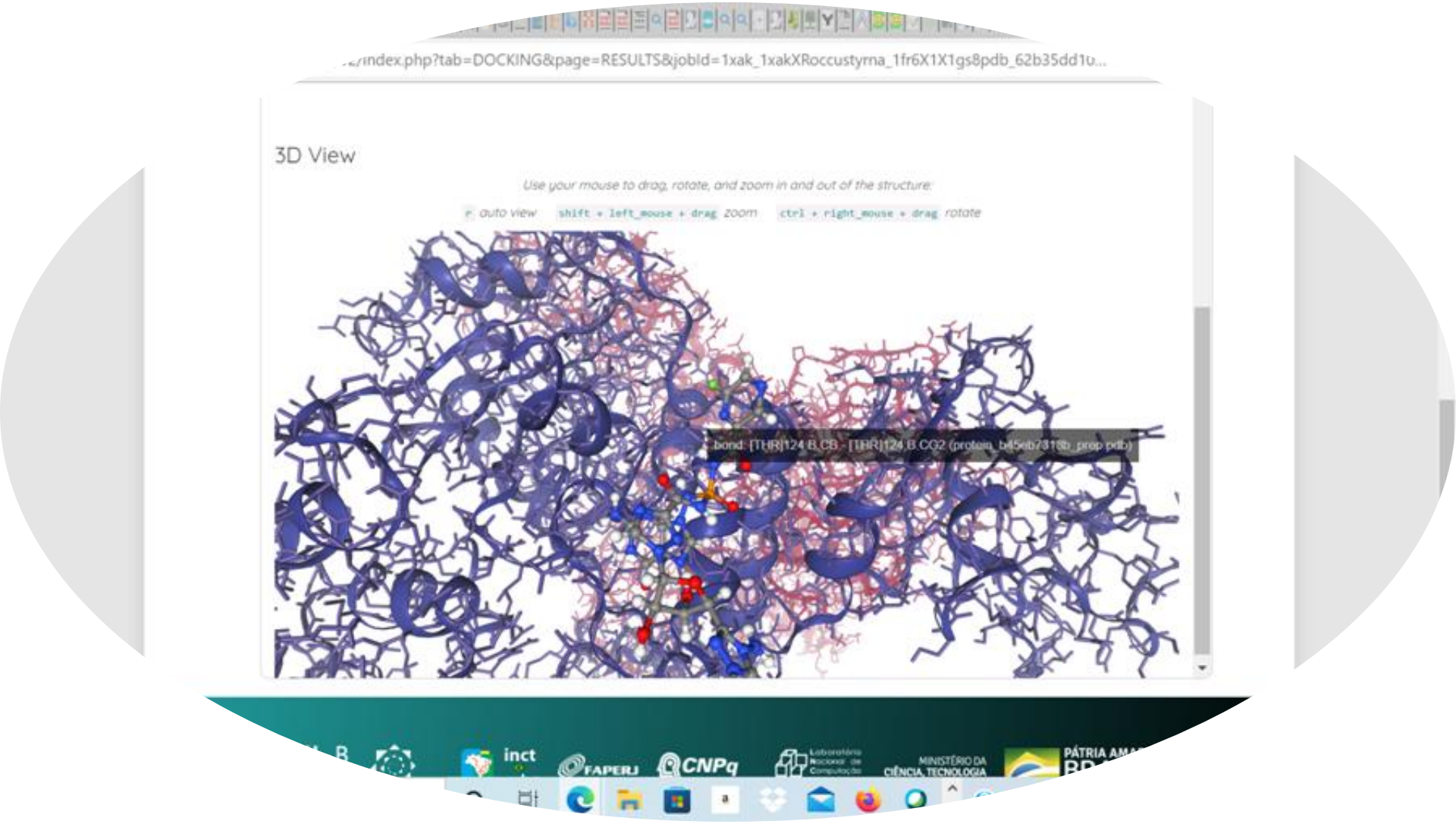
Table
3D View
« 1 2 3 »
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate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3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [THR]124.B.CB - [THR]124.B.CG2 (protein_b35db7818b_prep.pdb)
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA