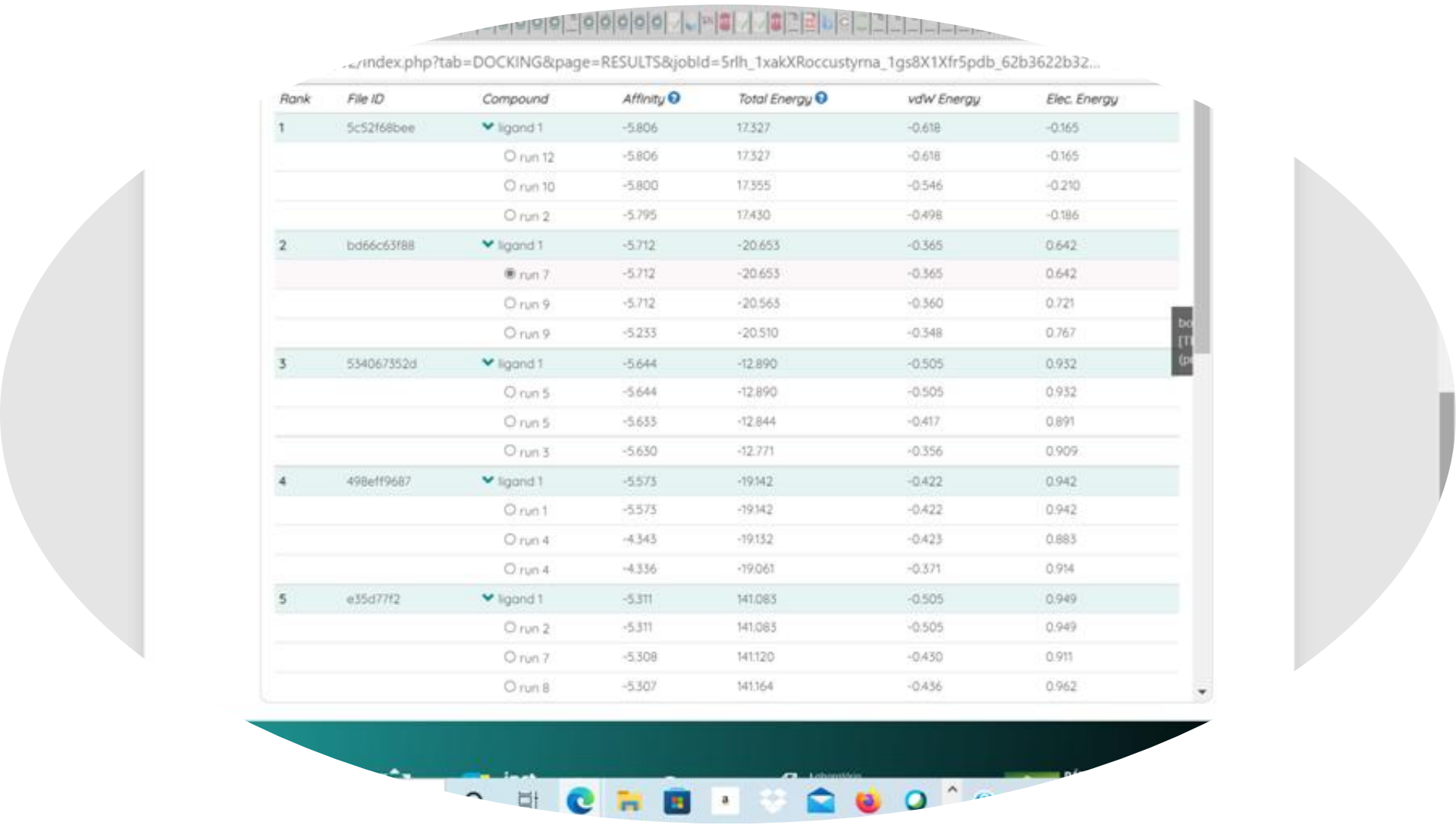
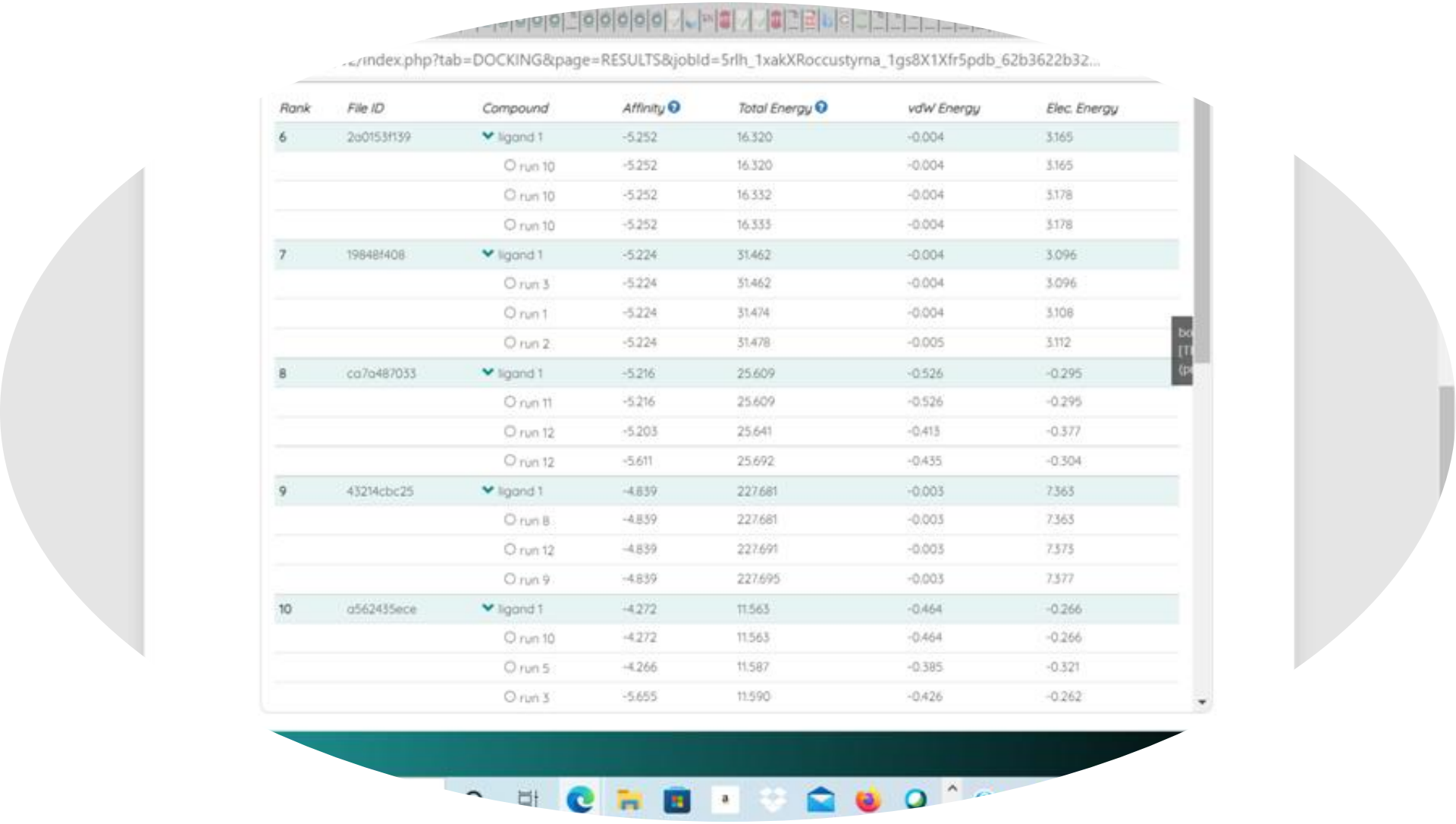
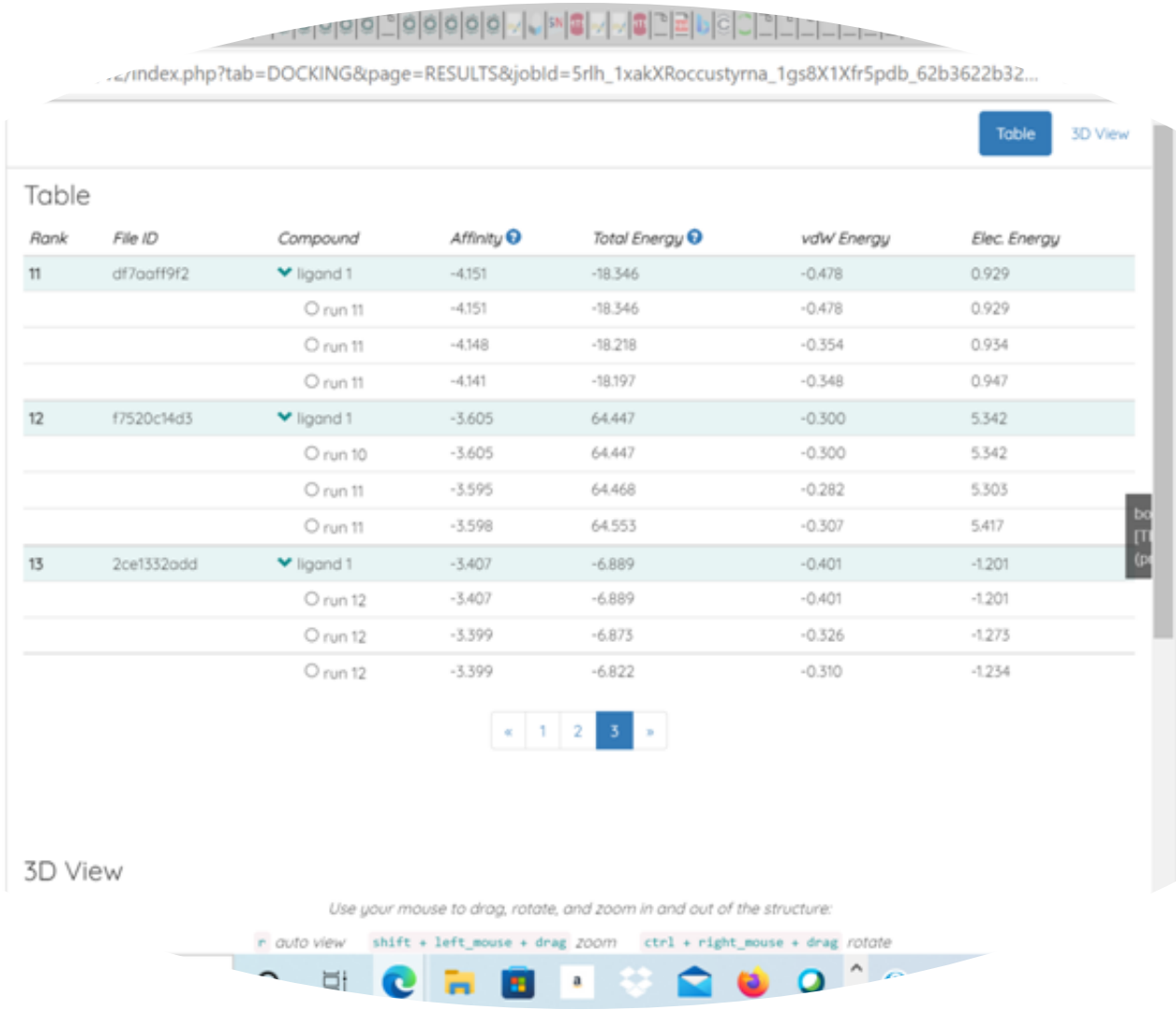
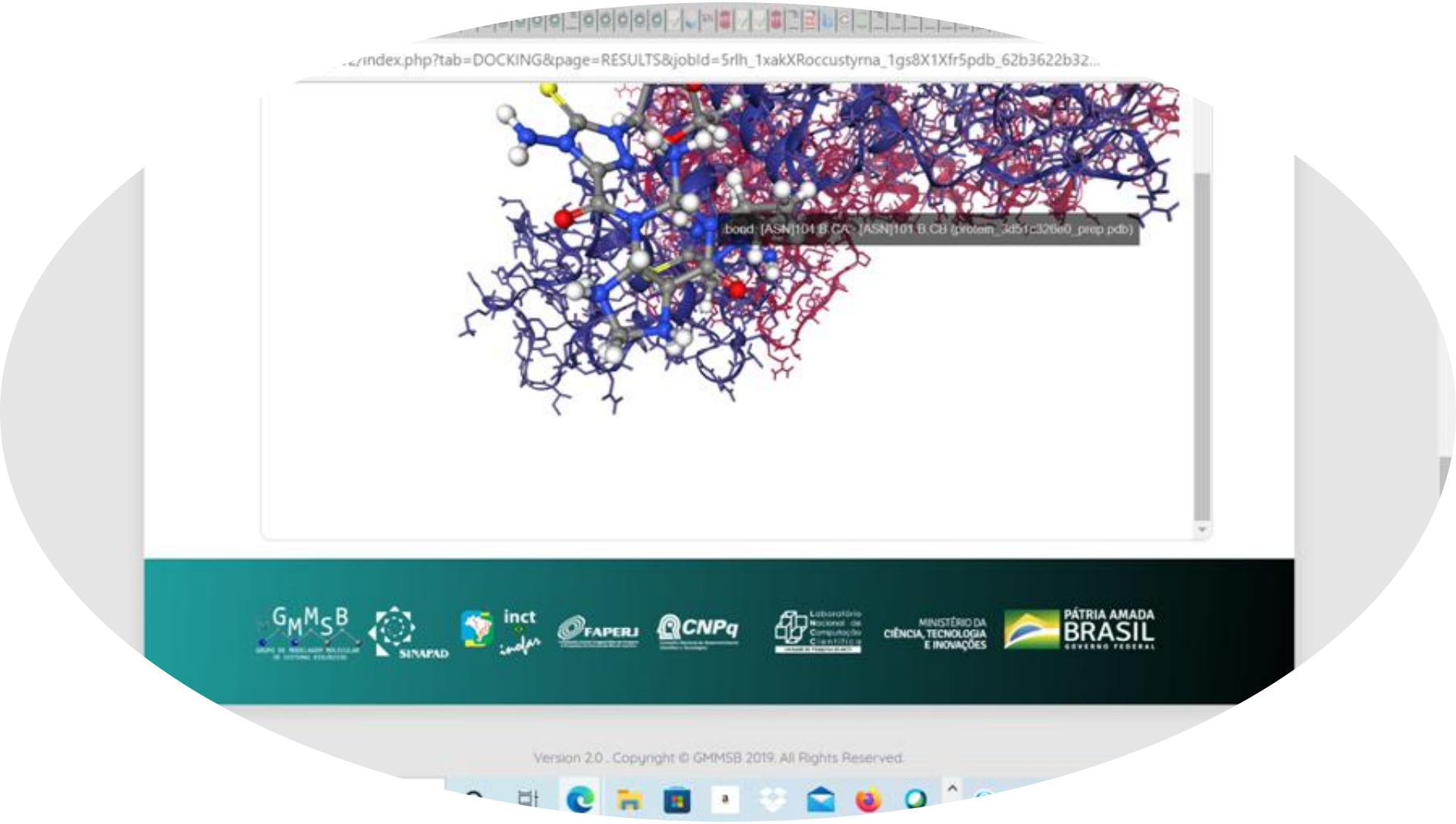


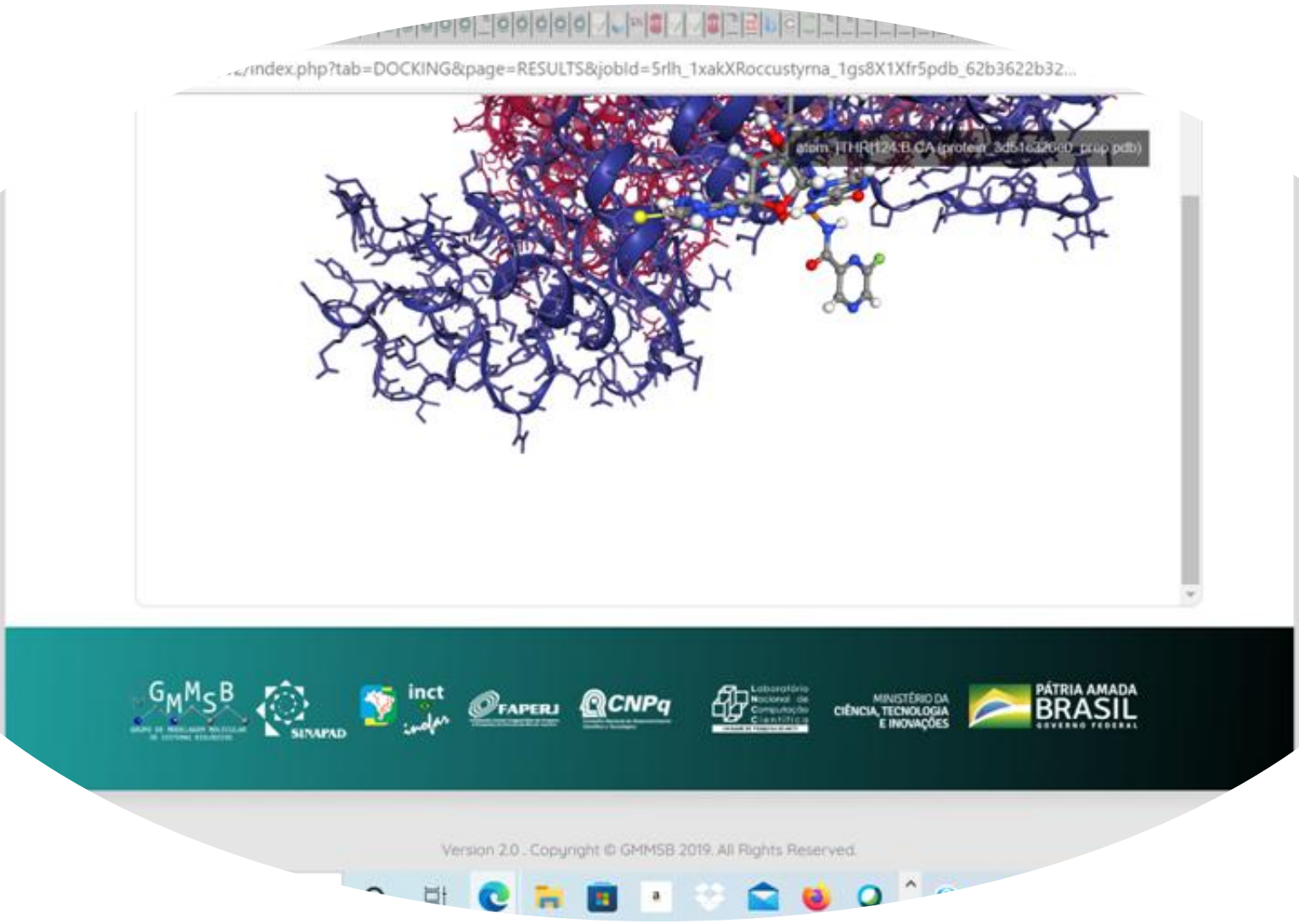
Rank	File ID	Compound	Affinity	Total Energy	vdW Energy	Elec. Energy
1	5c52f68bee	ligand 1	-5.806	17.327	-0.618	-0.165
		run 12	-5.806	17.327	-0.618	-0.165
		run 10	-5.800	17.355	-0.546	-0.210
		run 2	-5.795	17.430	-0.498	-0.186
2	bd66c63f88	ligand 1	-5.712	-20.653	-0.365	0.642
		run 7	-5.712	-20.653	-0.365	0.642
		run 9	-5.712	-20.565	-0.360	0.721
		run 9	-5.233	-20.510	-0.348	0.767
3	5340673520	ligand 1	-5.644	-12.890	-0.505	0.932
		run 5	-5.644	-12.890	-0.505	0.932
		run 5	-5.633	-12.844	-0.417	0.891
		run 3	-5.630	-12.771	-0.356	0.909
4	498ef19687	ligand 1	-5.573	-19.142	-0.422	0.942
		run 1	-5.573	-19.142	-0.422	0.942
		run 4	-4.343	-19.132	-0.423	0.883
		run 4	-4.336	-19.061	-0.371	0.914
5	e35d77f2	ligand 1	-5.311	141.085	-0.505	0.949
		run 2	-5.311	141.085	-0.505	0.949
		run 7	-5.308	141.120	-0.430	0.911
		run 8	-5.307	141.164	-0.436	0.962

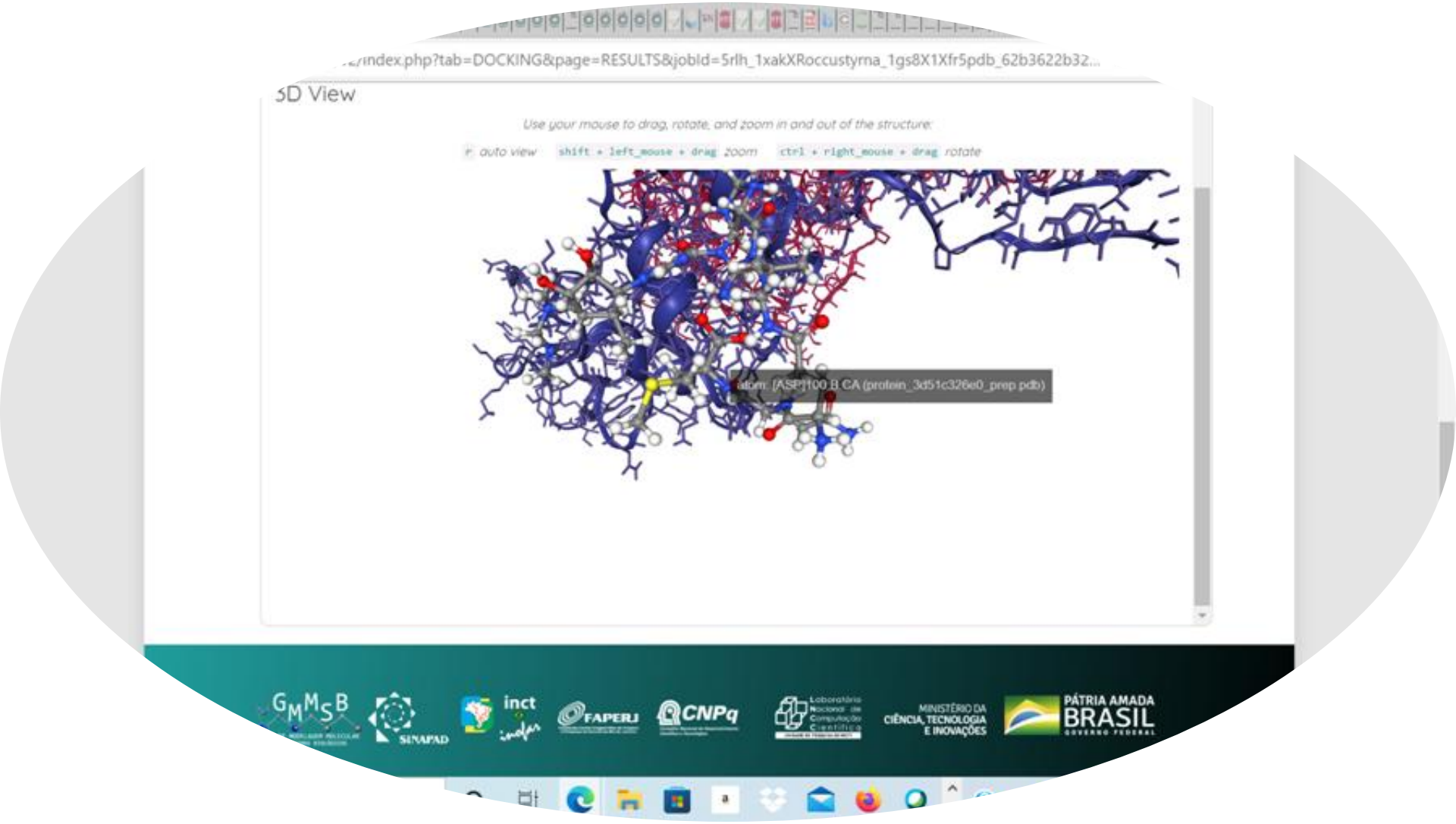


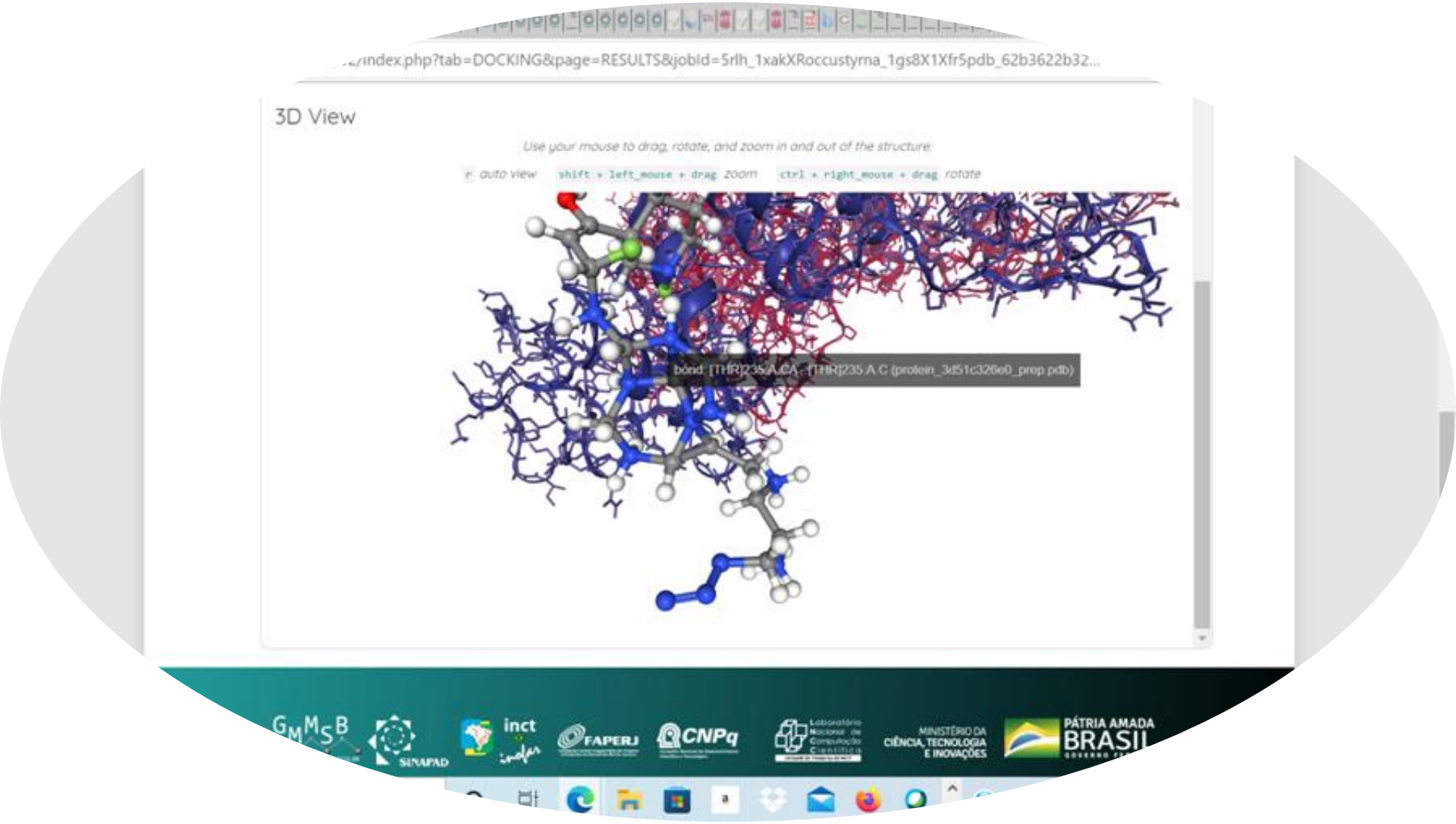
Rank	File ID	Compound	Affinity	Total Energy	vdW Energy	Elec. Energy
6	2a0153f139	ligand 1	-5.252	16.320	-0.004	3.165
		run 10	-5.252	16.320	-0.004	3.165
		run 10	-5.252	16.332	-0.004	3.178
		run 10	-5.252	16.333	-0.004	3.178
7	19848f408	ligand 1	-5.224	31.462	-0.004	3.096
		run 3	-5.224	31.462	-0.004	3.096
		run 1	-5.224	31.474	-0.004	3.108
		run 2	-5.224	31.478	-0.005	3.112
8	ca7a487033	ligand 1	-5.216	25.609	-0.526	-0.295
		run 11	-5.216	25.609	-0.526	-0.295
		run 12	-5.203	25.641	-0.413	-0.377
		run 12	-5.611	25.692	-0.435	-0.304
9	43214cbc25	ligand 1	-4.839	227.681	-0.003	7.365
		run 8	-4.839	227.681	-0.003	7.365
		run 12	-4.839	227.691	-0.003	7.375
		run 9	-4.839	227.695	-0.003	7.377
10	a562435ece	ligand 1	-4.272	11.563	-0.464	-0.266
		run 10	-4.272	11.563	-0.464	-0.266
		run 5	-4.266	11.587	-0.385	-0.321
		run 3	-5.655	11.590	-0.426	-0.262

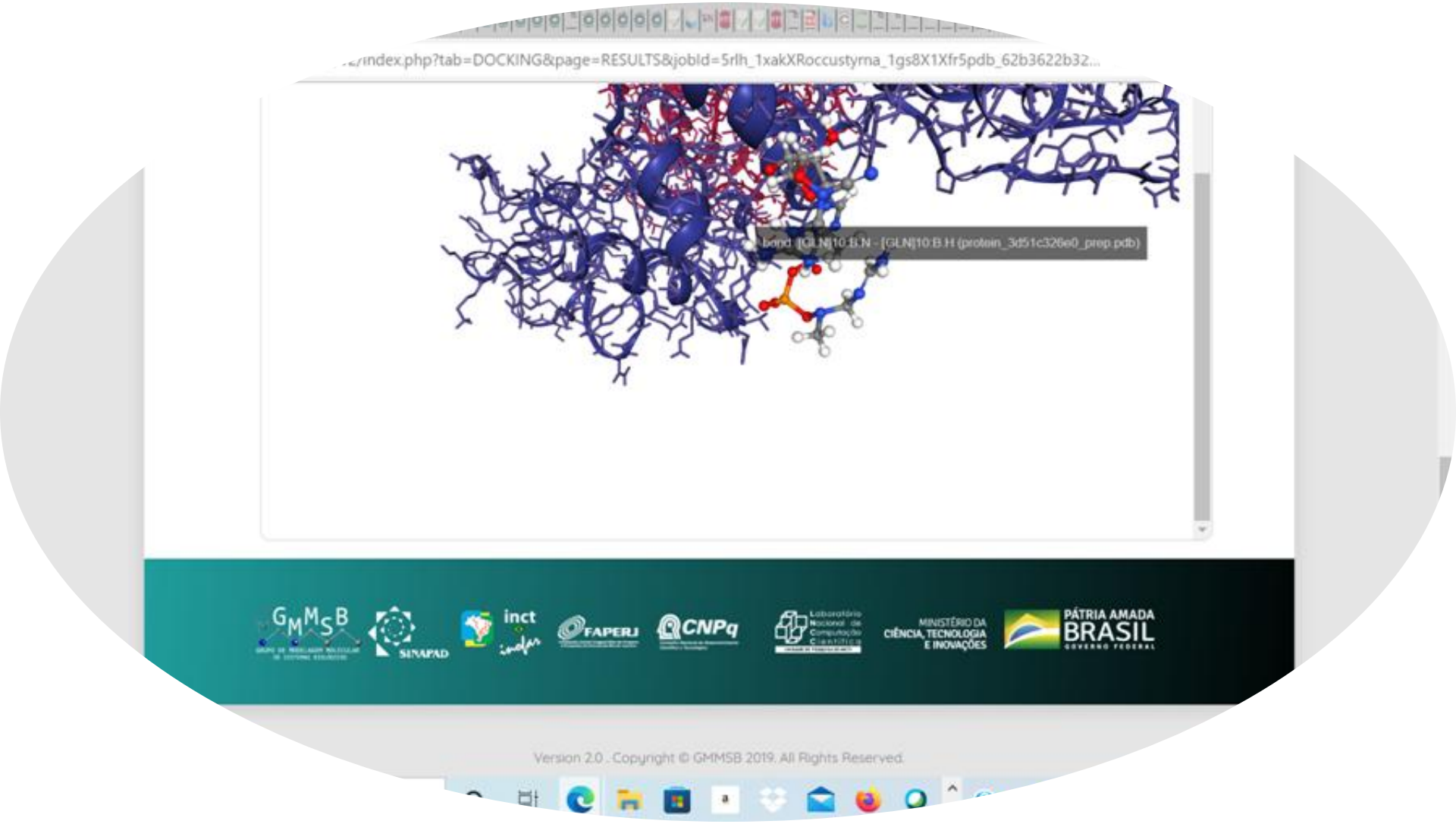

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
Table
3D View
Table
Rank File ID Compound Affinity Total Energy vdW Energy Elec. Energy
11 df7aaff9f2 ligand 1 -4.151 -18.346 -0.478 0.929
run 11 -4.151 -18.346 -0.478 0.929
run 11 -4.148 -18.218 -0.354 0.934
run 11 -4.141 -18.197 -0.348 0.947
12 f7520c14d3 ligand 1 -3.605 64.447 -0.300 5.342
run 10 -3.605 64.447 -0.300 5.342
run 11 -3.595 64.468 -0.282 5.303
run 11 -3.598 64.553 -0.307 5.417
13 2ce1332add ligand 1 -3.407 -6.889 -0.401 -1.201
run 12 -3.407 -6.889 -0.401 -1.201
run 12 -3.399 -6.873 -0.326 -1.273
run 12 -3.399 -6.822 -0.310 -1.234
« 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

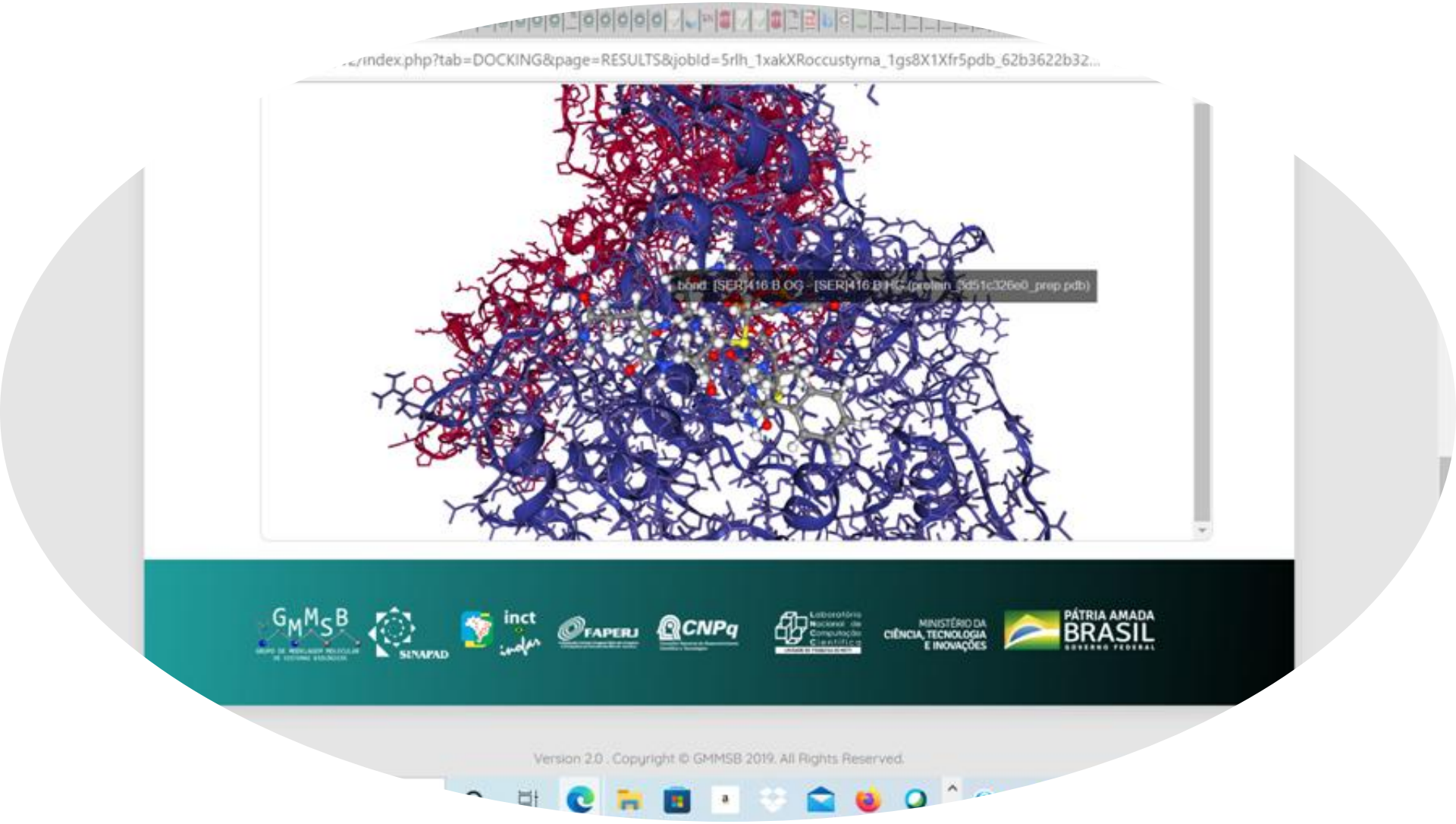

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
bond: [ASN]104:B:CA - [ASN]101:B:CB (protein_3d51c326e0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
GOVERNO FEDERAL
Version 2.0 . Copyright © GMMSB 2019. All Rights Reserved.

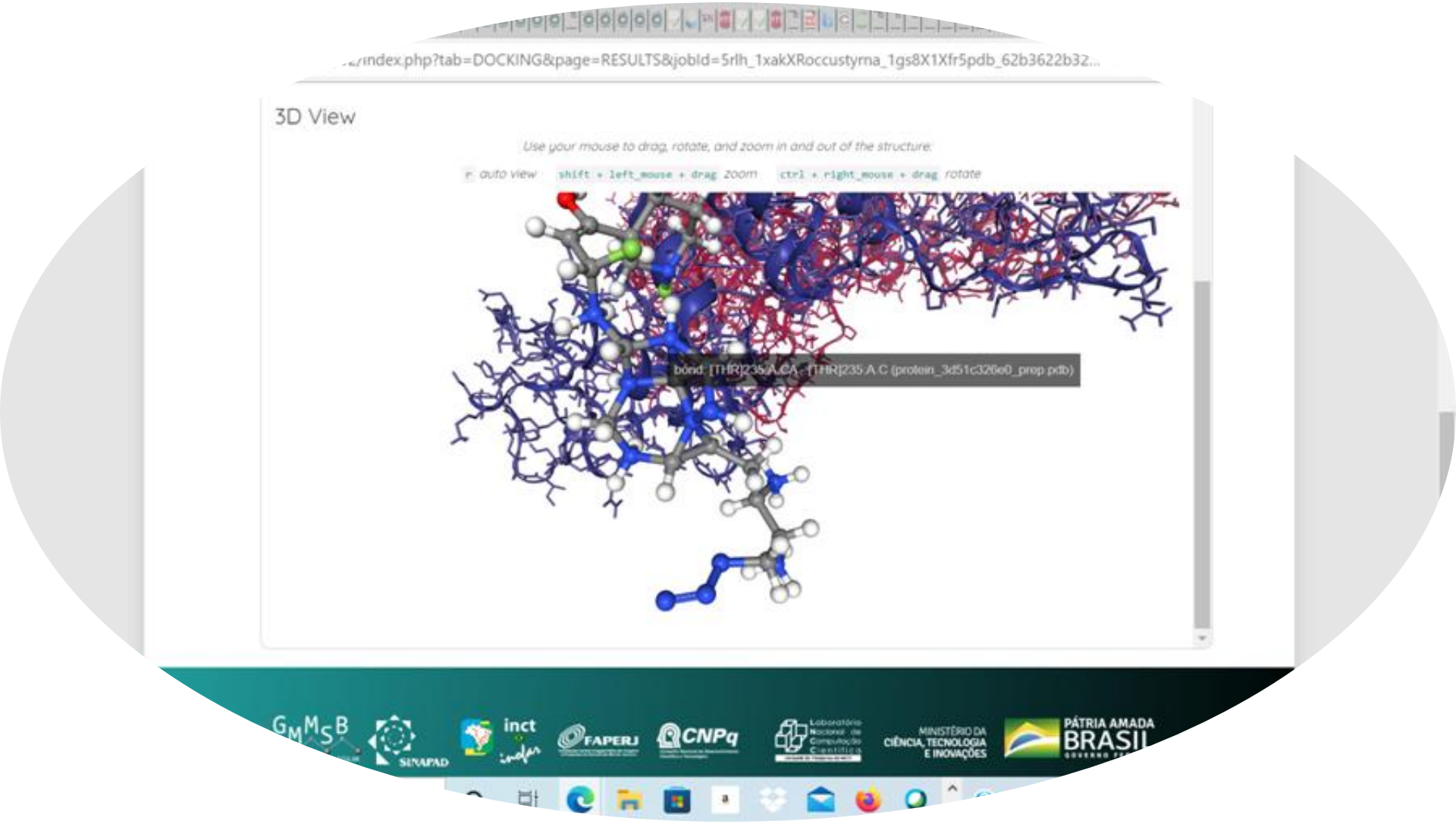

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
GOVERNO FEDERAL
Version 2.0 . Copyright © GMMSB 2019. All Rights Reserved.

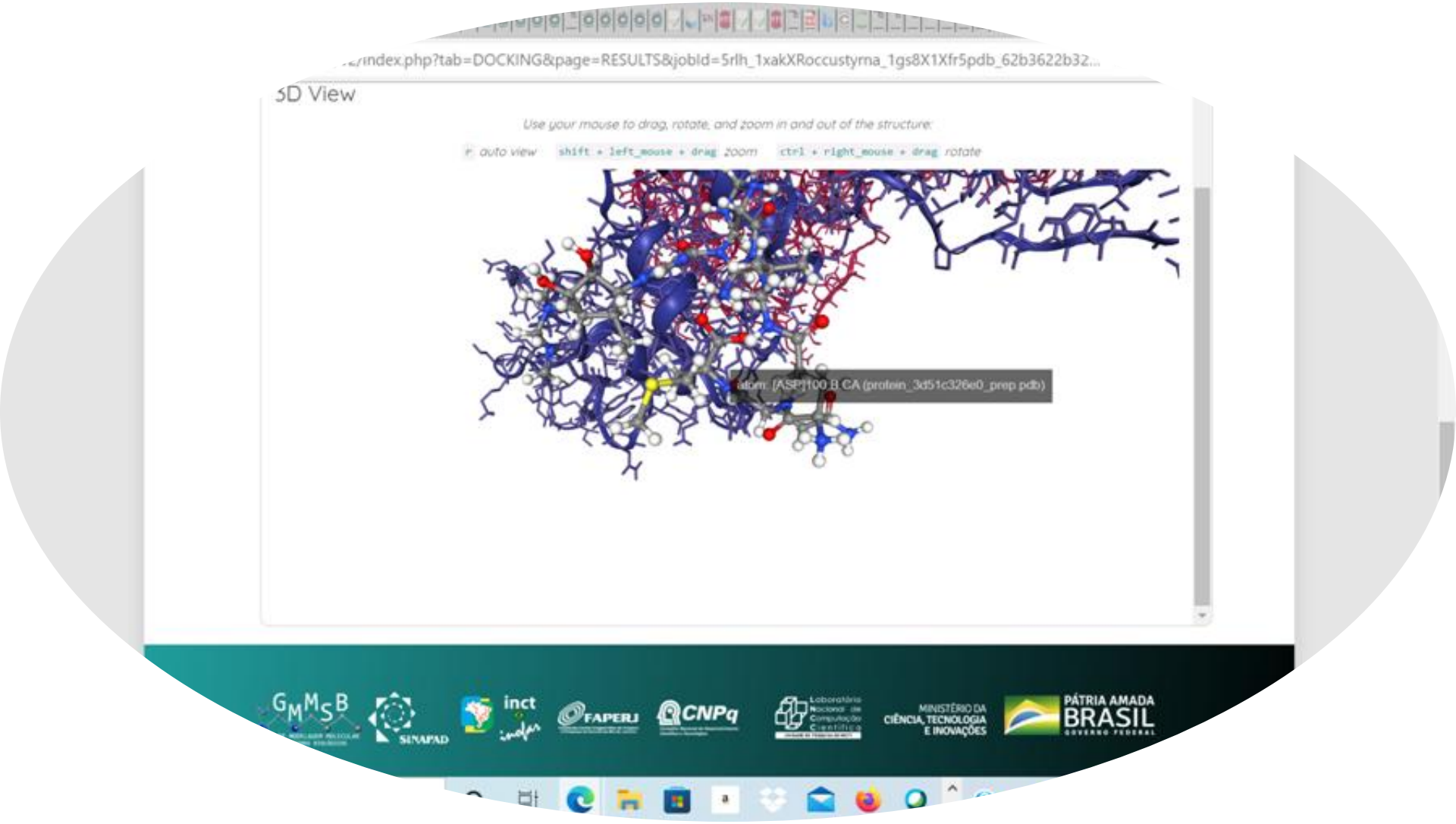

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
atom: [ASP]100.B.CA (protein_3d51c326e0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
GOVERNO FEDERAL

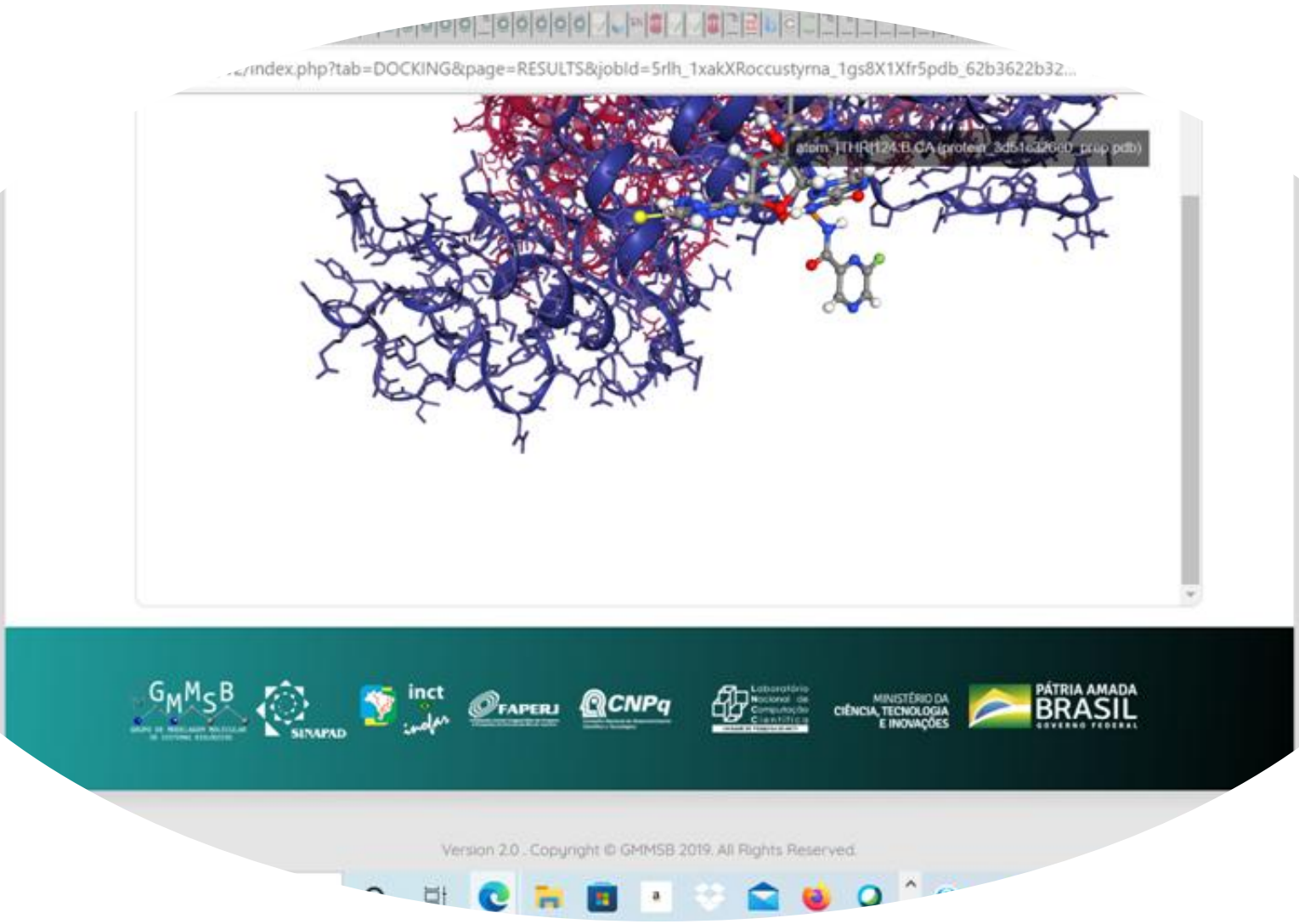

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [THR]235:A.CA - [THR]235:A.C (protein_3d51c326e0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL

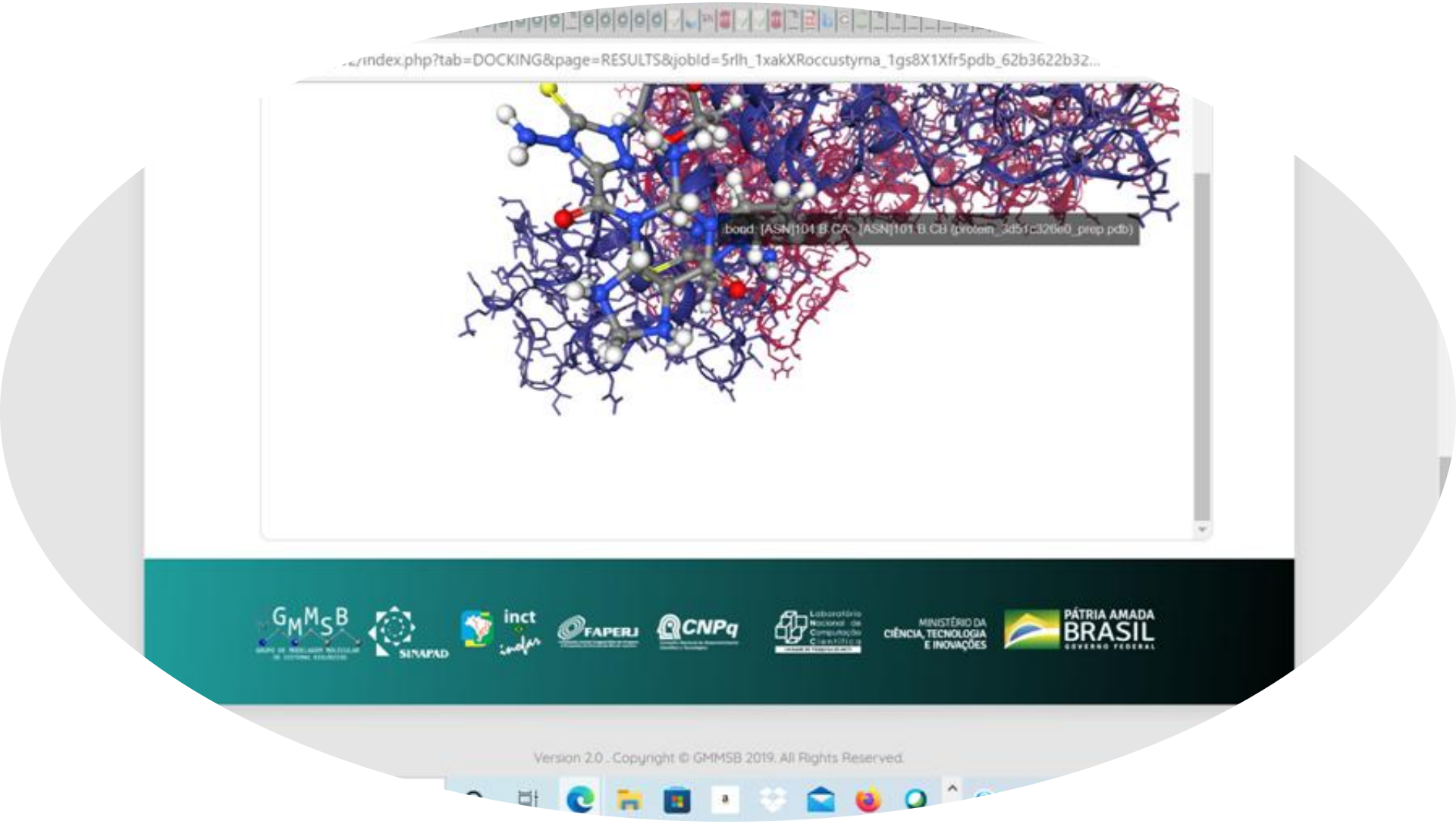

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
bond: [GLN]10:B:N - [GLN]10:B:H (protein_3d51c326e0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
GOVERNO FEDERAL
Version 2.0 . Copyright © GMMSB 2019. All Rights Reserved.

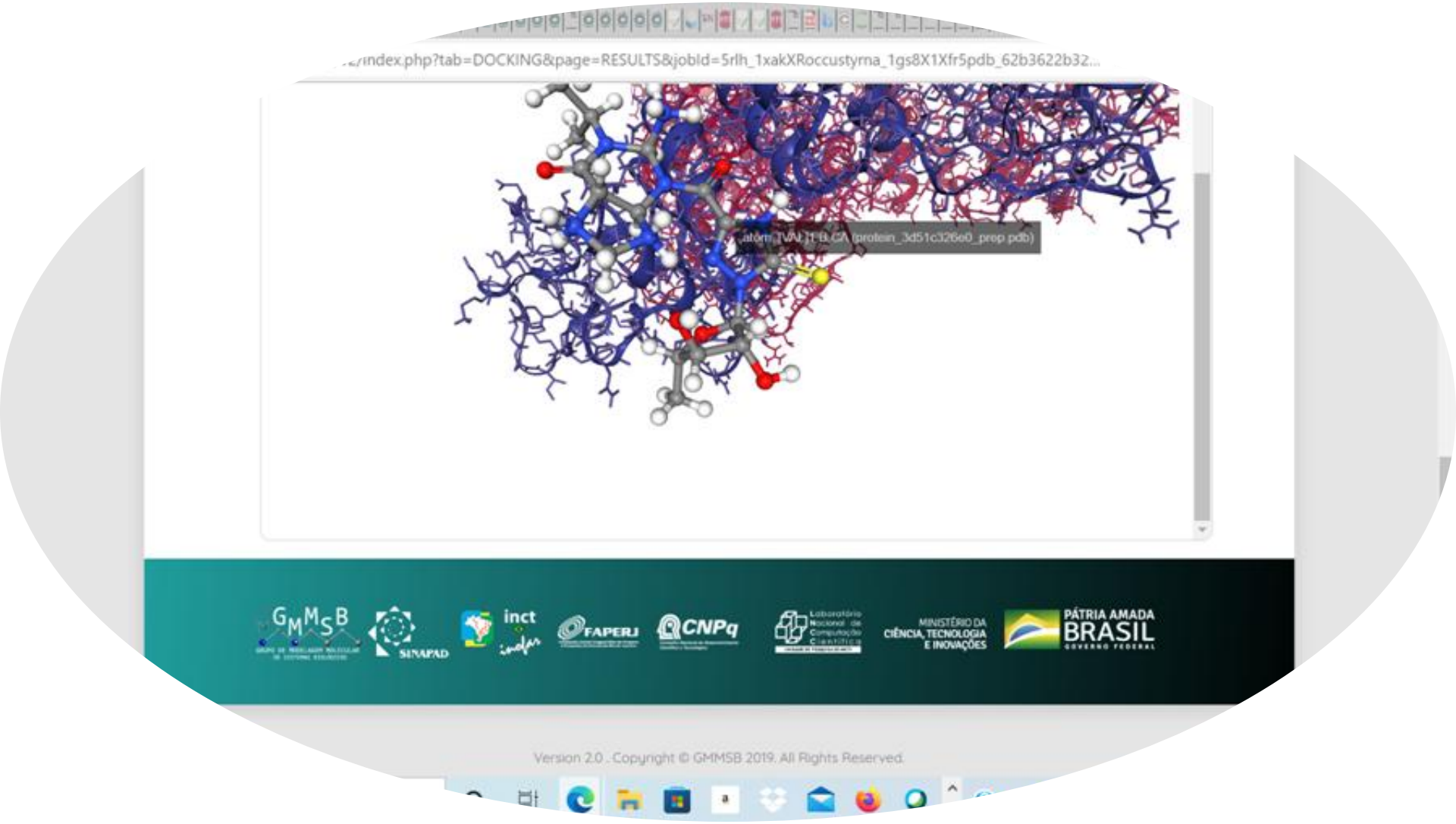

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
bond: [SER]416:B:OG - [SER]416:B:HG (prelim_5d51c326e0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
GOVERNO FEDERAL
Version 2.0 . Copyright © GMMSB 2019. All Rights Reserved.

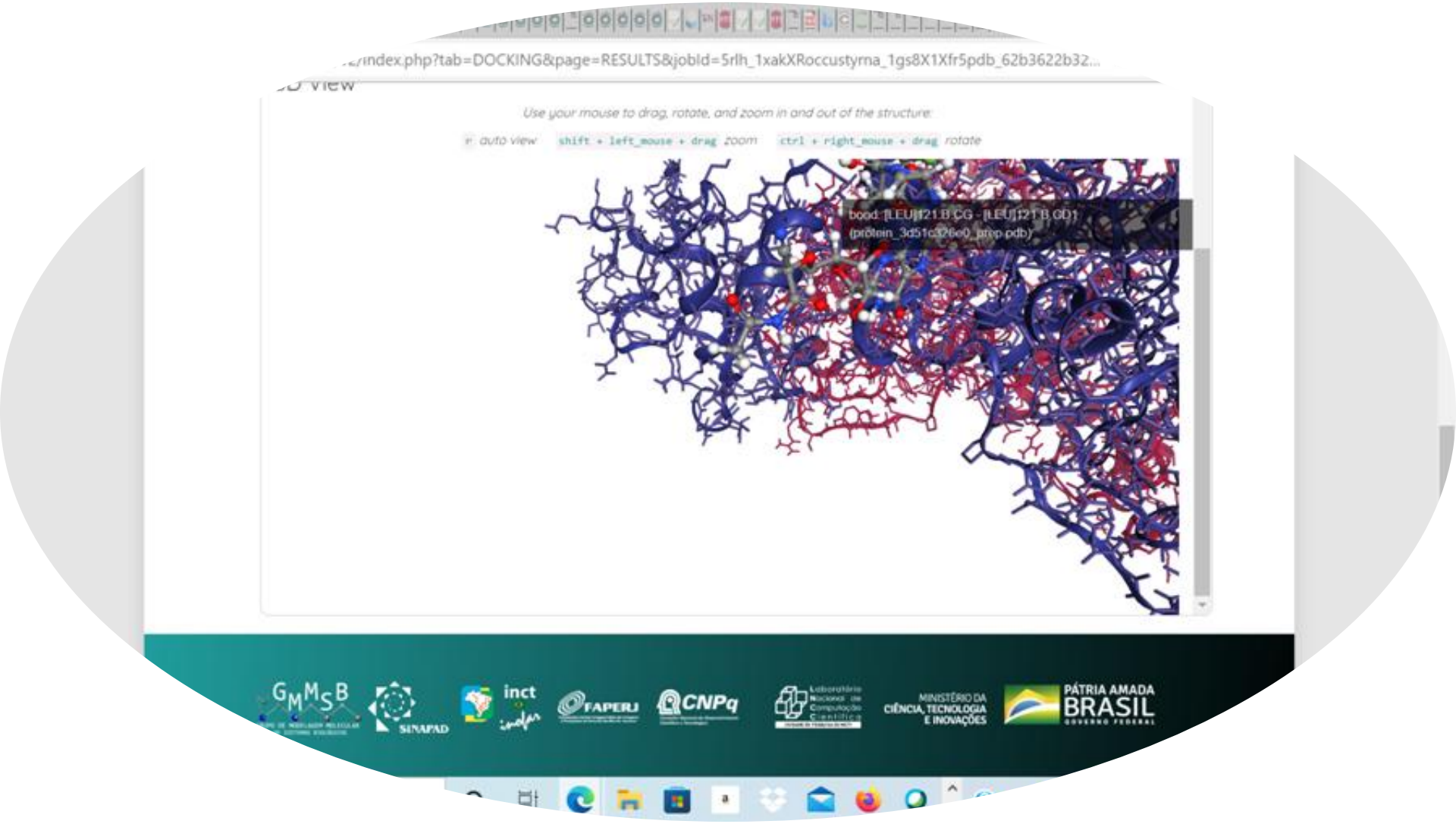

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [THR]235:A.CA - [THR]235:A.C (protein_3d51c326e0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL

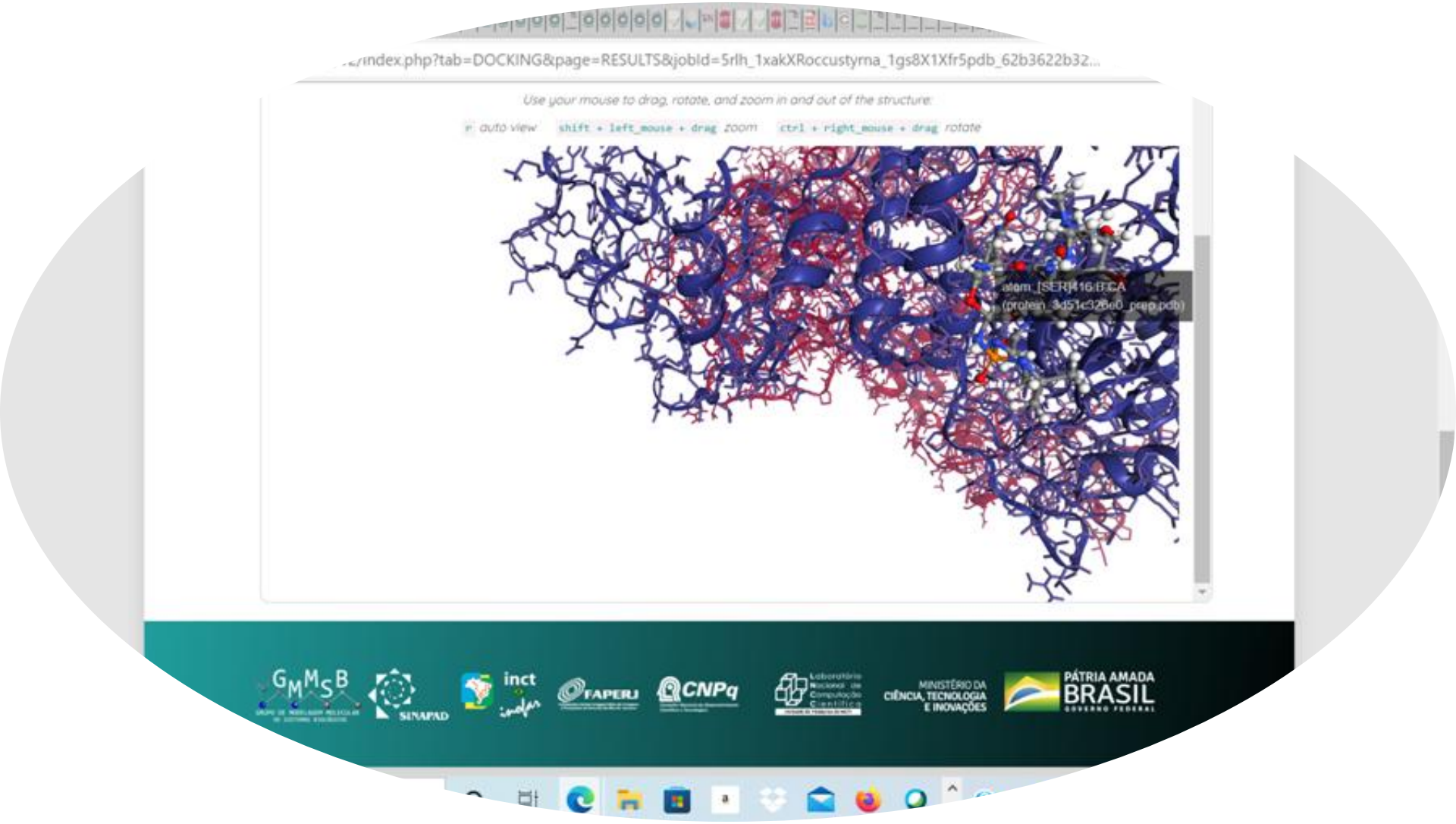

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
5D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
atom: [ASP]100.B.CA (protein_3d51c326e0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
GOVERNO FEDERAL

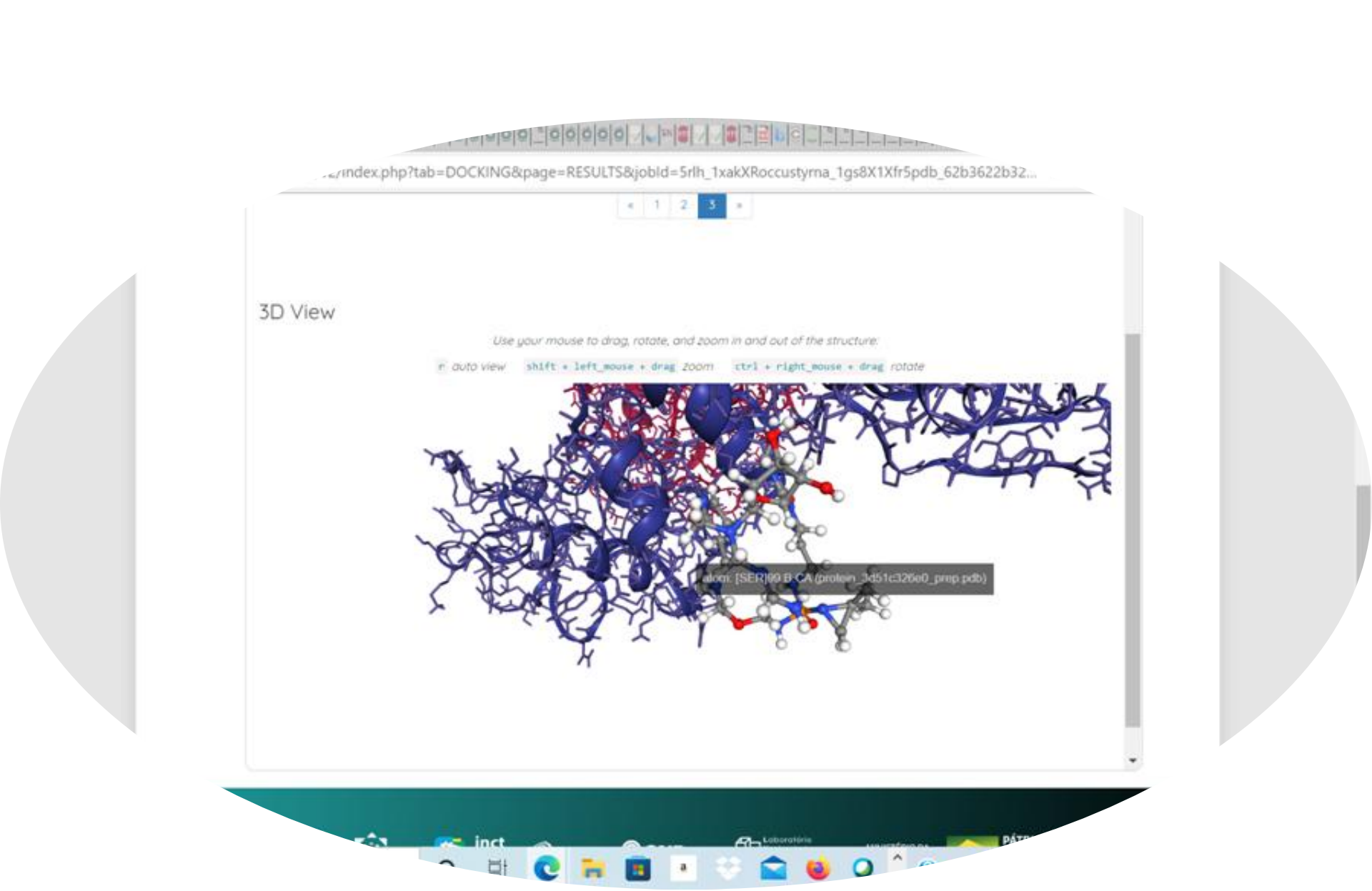

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
GOVERNO FEDERAL
Version 2.0 . Copyright © GMMSB 2019. All Rights Reserved.

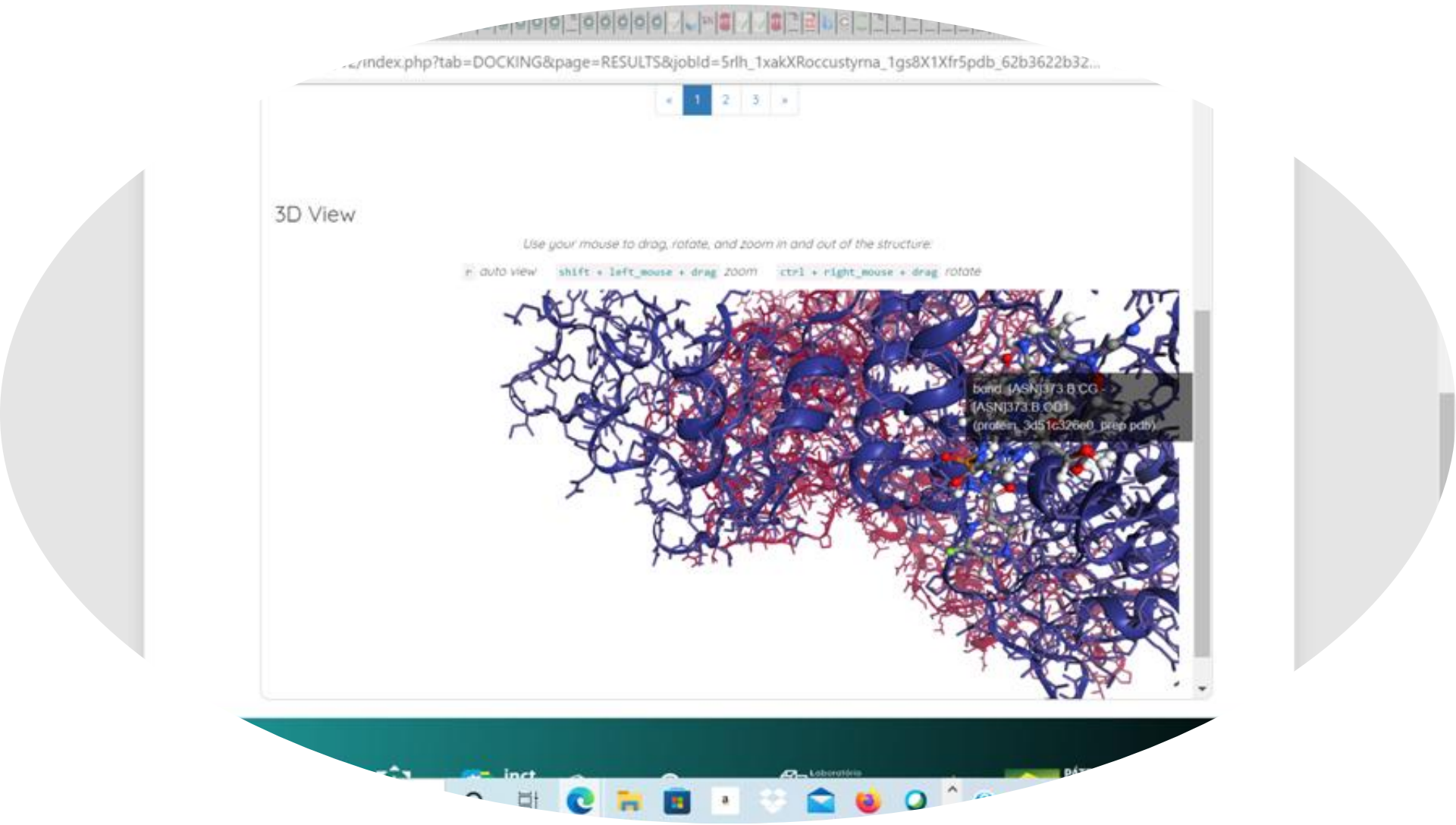

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
bond: [ASN]104:B:CA - [ASN]101:B:CB (protein_3d51c326e0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
GOVERNO FEDERAL
Version 2.0 . Copyright © GMMSB 2019. All Rights Reserved.

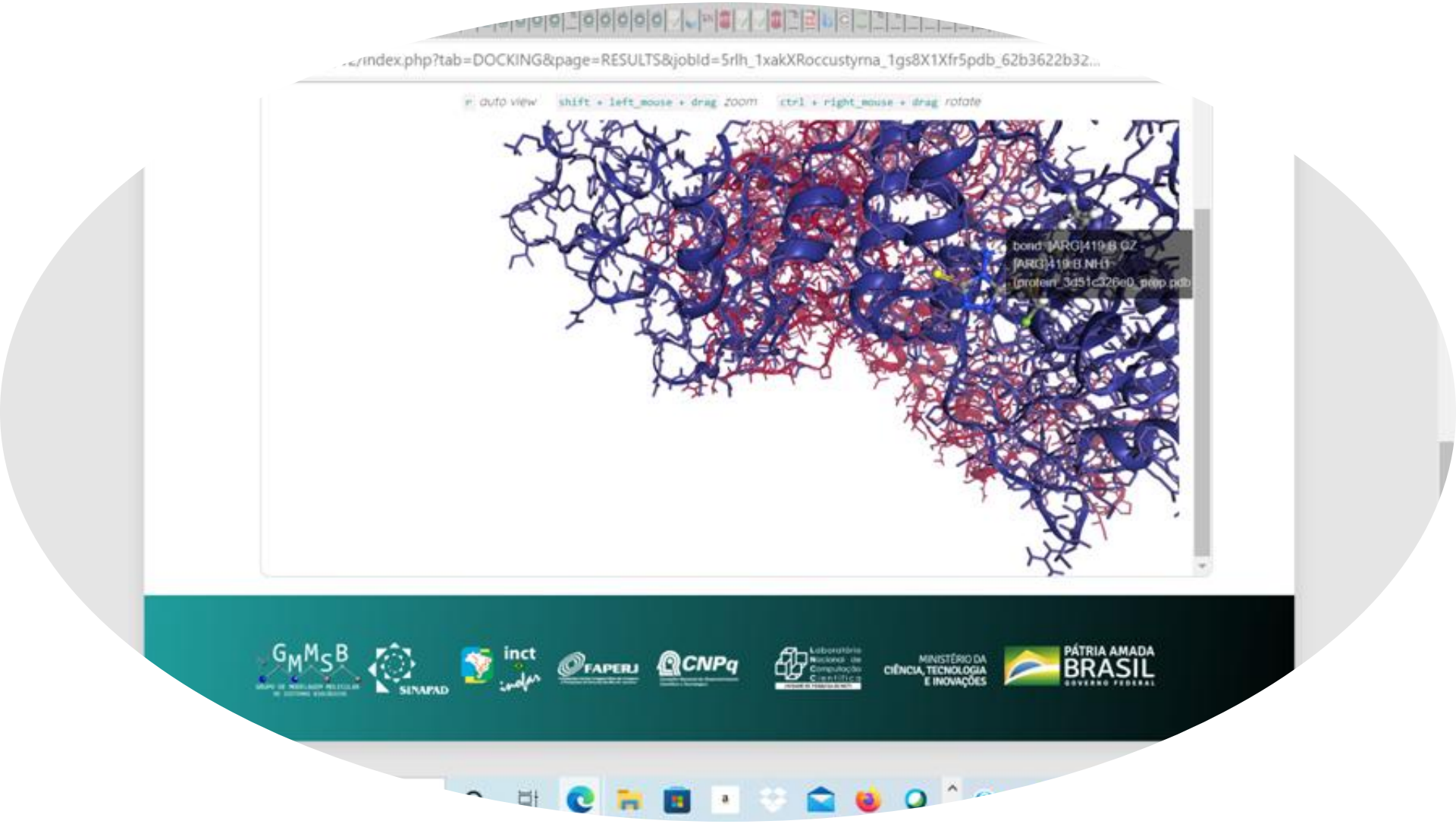

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
Version 2.0 . Copyright © GMMSB 2019. All Rights Reserved.

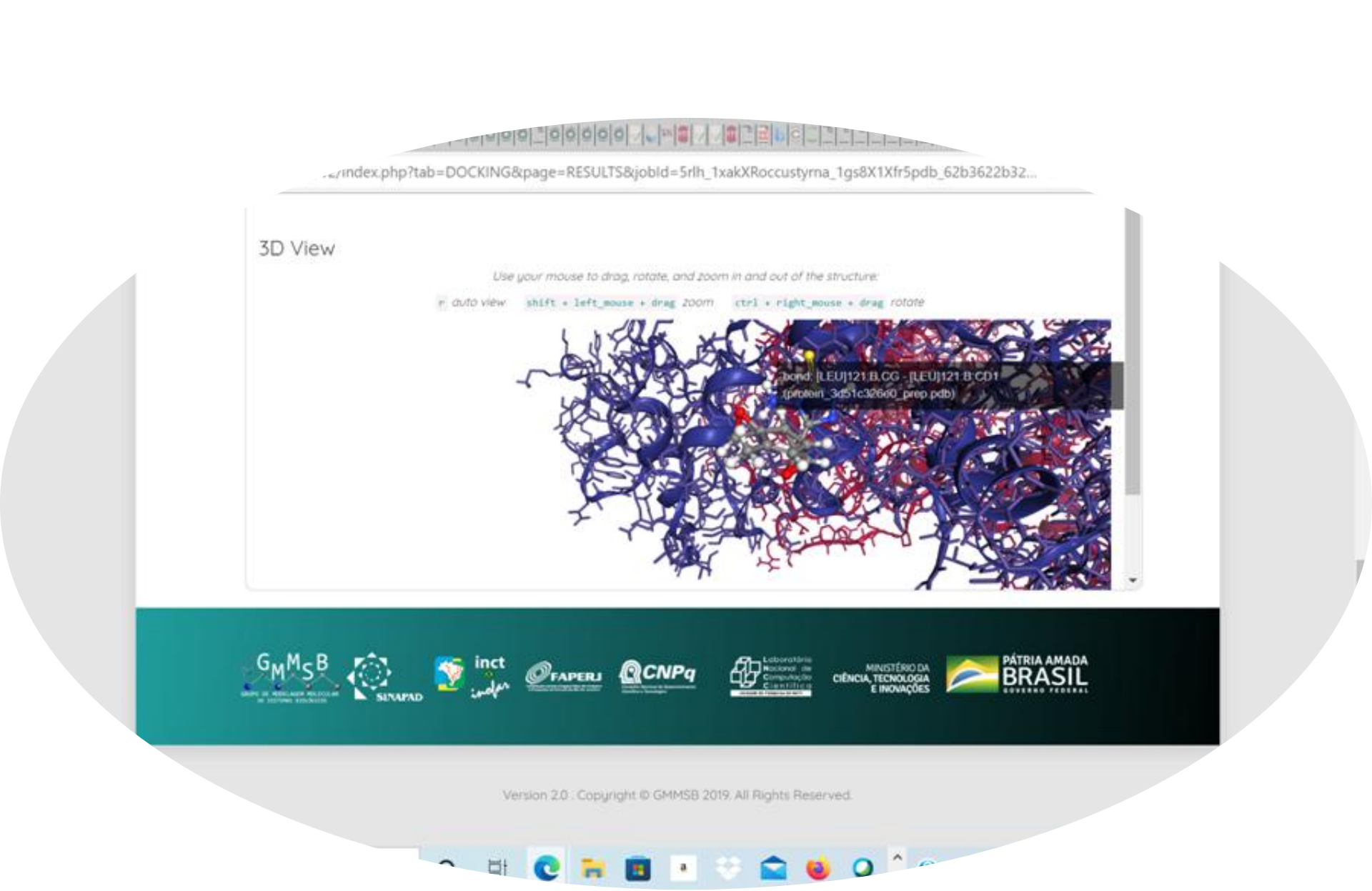

index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [LEU]121.B.CG - [LEU]121.B.CD1
(protein_3d51c326e0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
GOVERNO FEDERAL


index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
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
atom: [SER]416:B:CA
(protein_3d51c326e0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL


index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
« 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=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
« 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.CG -
(ASN)373.B.OD1
(protein_3d51c326e0_prep.pdb)


index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond [ARG]419:B.CZ
[ARG]419:B.NH1
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL


index.php?tab=DOCKING&page=RESULTS&jobId=5rlh_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b3622b32...
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: [LEU]121.B.CG - [LEU]121.B.CD1
(protein_3d51c326d0_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÕES
PÁTRIA AMADA BRASIL
GOVERNO FEDERAL
Version 2.0 . Copyright © GMMSB 2019. All Rights Reserved.