index.php?tab=DOCKING&page=RESULTS&jobId=5rem_1xakXRoccustyrna_gs6X1Xpdb_62b443670990
Rank File ID Compound Affinity Total Energy vdW Energy Elec. Energy
1 1d0aa1d25a ligand 1 -7.791 -53.924 -18.678 -29.784
run 2 -7.791 -53.924 -18.678 -29.784
run 3 -7.714 -55.618 -17.623 -30.280
run 8 -7.786 -50.040 -16.350 -31.061
2 6fcbb8e547 ligand 1 -7.565 -5.044 -22.408 -11.859
run 3 -7.565 -5.044 -22.408 -11.859
run 7 -7.811 -4.410 -20.917 -12.332
run 7 -7.694 -4.271 -18.740 -13.742
3 db51c934a6 ligand 1 -7.555 -48.956 -24.056 -19.974
run 7 -7.555 -48.956 -24.056 -19.974
run 7 -7.374 -48.576 -22.929 -24.106
run 7 -7.528 -47.909 -25.475 -21.154
4 533e42957d ligand 1 -7.539 107.920 -18.831 -17.635
run 5 -7.539 107.920 -18.831 -17.635
run 12 -7.369 108.984 -12.374 -23.028
run 10 -6.995 110.644 -5.460 -33.422
5 7888f0b ligand 1 -7.326 -18.103 -19.360 -12.281
run 1 -7.326 -18.103 -19.360 -12.281
run 1 -7.163 -17.683 -14.766 -19.404
run 3 -7.122 -17.575 -16.996 -15.300

Rank	File ID	Compound	Affinity	Total Energy	vdW Energy	Elec. Energy
6	1dfc0b3f53	ligand 1	-7.310	-1.601	-11.901	-8.362
		run 3	-7.310	-1.601	-11.901	-8.362
		run 10	-7.100	-1.294	-9.198	-10.787
		run 6	-7.148	-1.154	-10.264	-9.272
7	ae4c410e95	ligand 1	-7.203	172.184	-8.666	-40.155
		run 5	-7.203	172.184	-8.666	-40.155
		run 9	-7.427	175.074	-10.467	-39.198
		run 9	-7.111	175.419	-9.656	-39.835
8	ed95926d60	ligand 1	-7.147	41.354	-23.564	-19.204
		run 2	-7.147	41.354	-23.564	-19.204
		run 2	-7.131	41.500	-15.007	-17.502
		run 2	-7.052	42.194	-20.789	-19.082
9	6022ed281f	ligand 1	-7.117	-1.400	-12.407	-21.322
		run 12	-7.117	-1.400	-12.407	-21.322
		run 12	-7.074	-0.388	-12.675	-19.699
		run 10	-6.738	-0.157	-12.370	-17.851
10	055f7a2bc4	ligand 1	-7.047	-13.539	-13.168	-22.883
		run 6	-7.047	-13.539	-13.168	-22.883
		run 7	-7.180	-12.416	-15.833	-29.071
		run 7	-7.253	-11.710	-13.303	-31.234

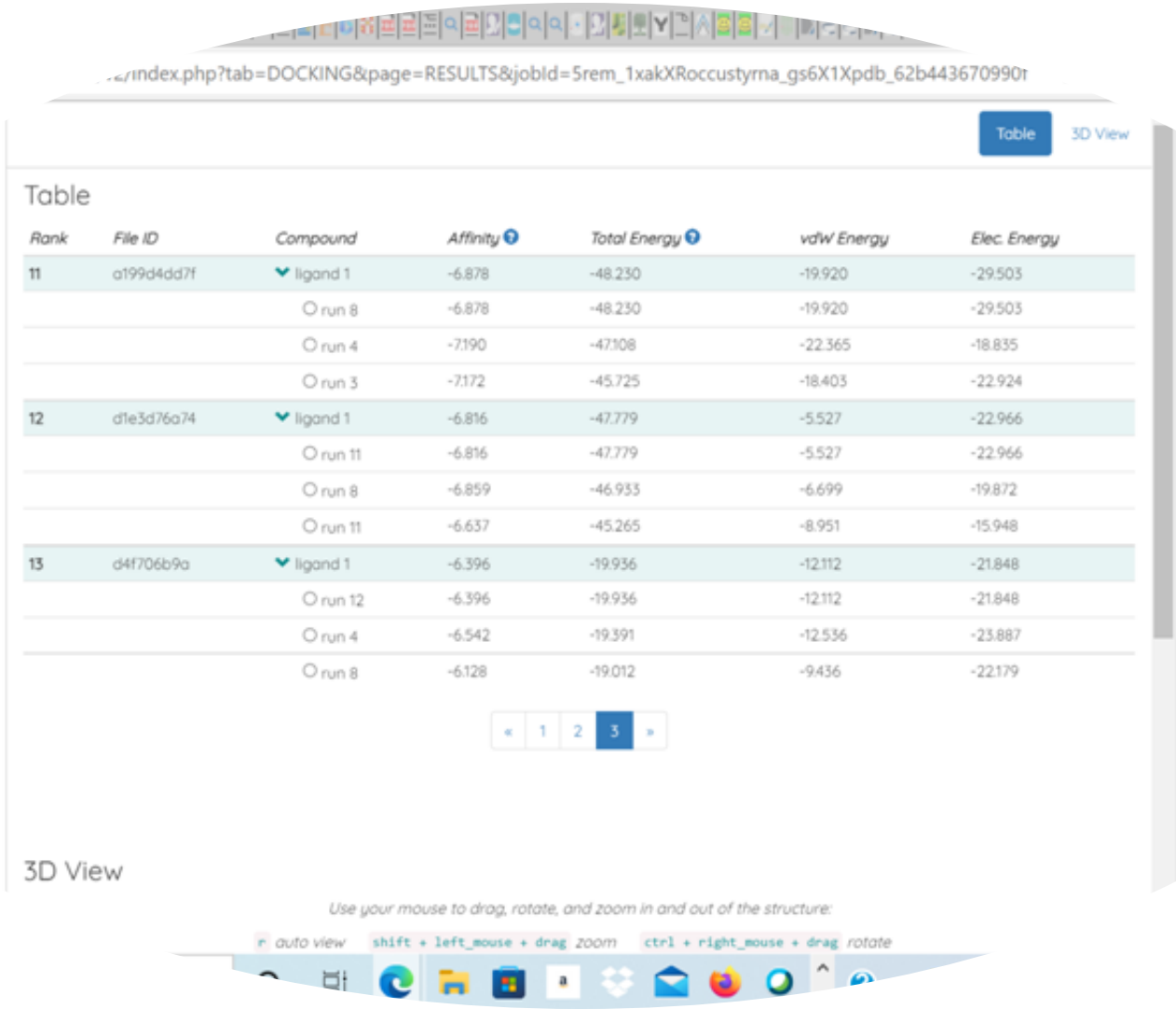
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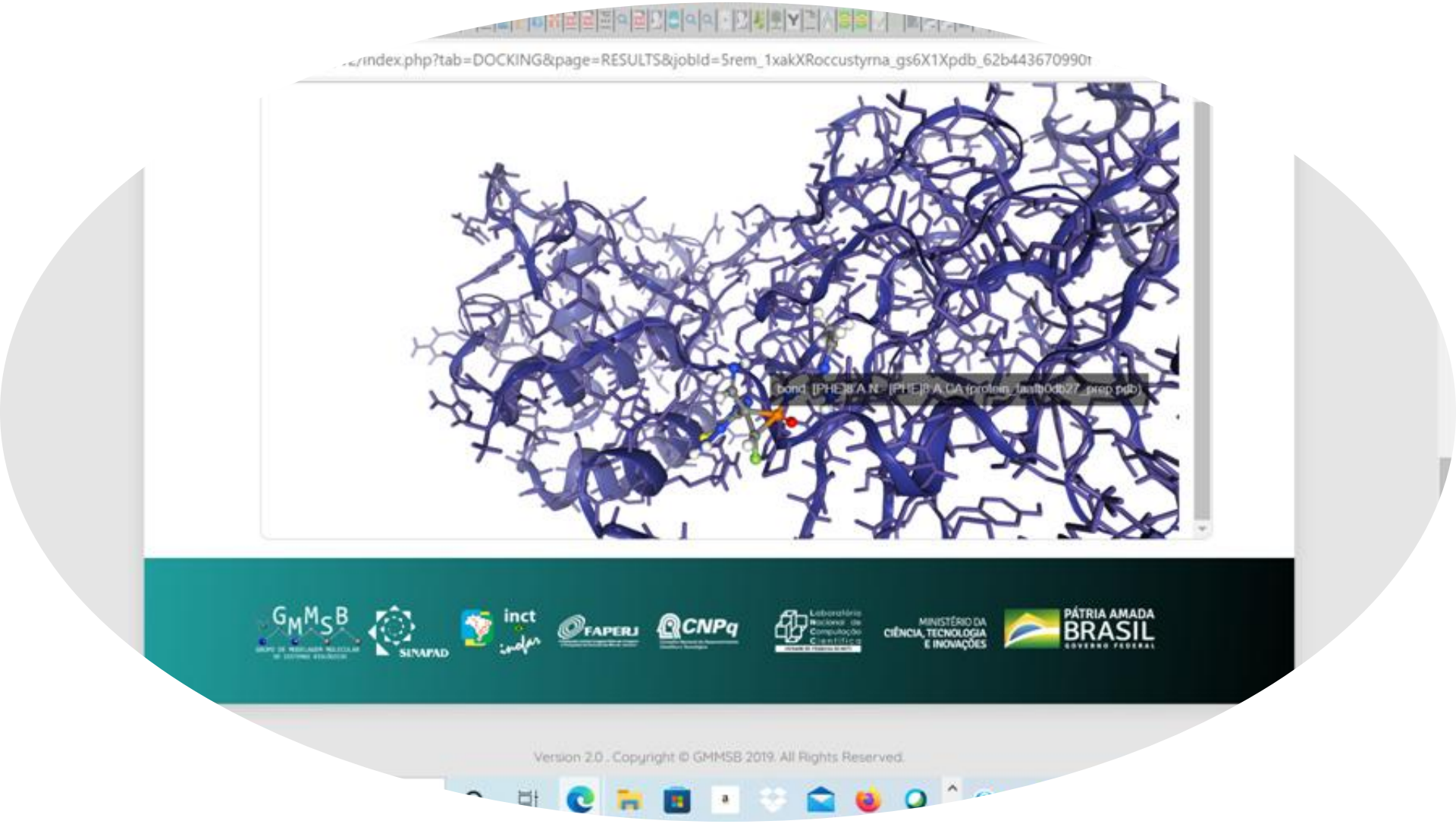
Table
3D View
Table
Rank File ID Compound Affinity Total Energy vdW Energy Elec. Energy
11 a199d4dd7f ligand 1 -6.878 -48.230 -19.920 -29.503
run 8 -6.878 -48.230 -19.920 -29.503
run 4 -7.190 -47.108 -22.365 -18.835
run 3 -7.172 -45.725 -18.403 -22.924
12 d1e3d76a74 ligand 1 -6.816 -47.779 -5.527 -22.966
run 11 -6.816 -47.779 -5.527 -22.966
run 8 -6.859 -46.933 -6.699 -19.872
run 11 -6.637 -45.265 -8.951 -15.948
13 d4f706b9a ligand 1 -6.396 -19.936 -12.112 -21.848
run 12 -6.396 -19.936 -12.112 -21.848
run 4 -6.542 -19.391 -12.536 -23.887
run 8 -6.128 -19.012 -9.436 -22.179
« 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=5rem_1xakXRoccustyrna_gs6X1Xpdb_62b443670990
bond: [PHE]8:A:N - [PHE]8:A:CA (protein_fastDock27_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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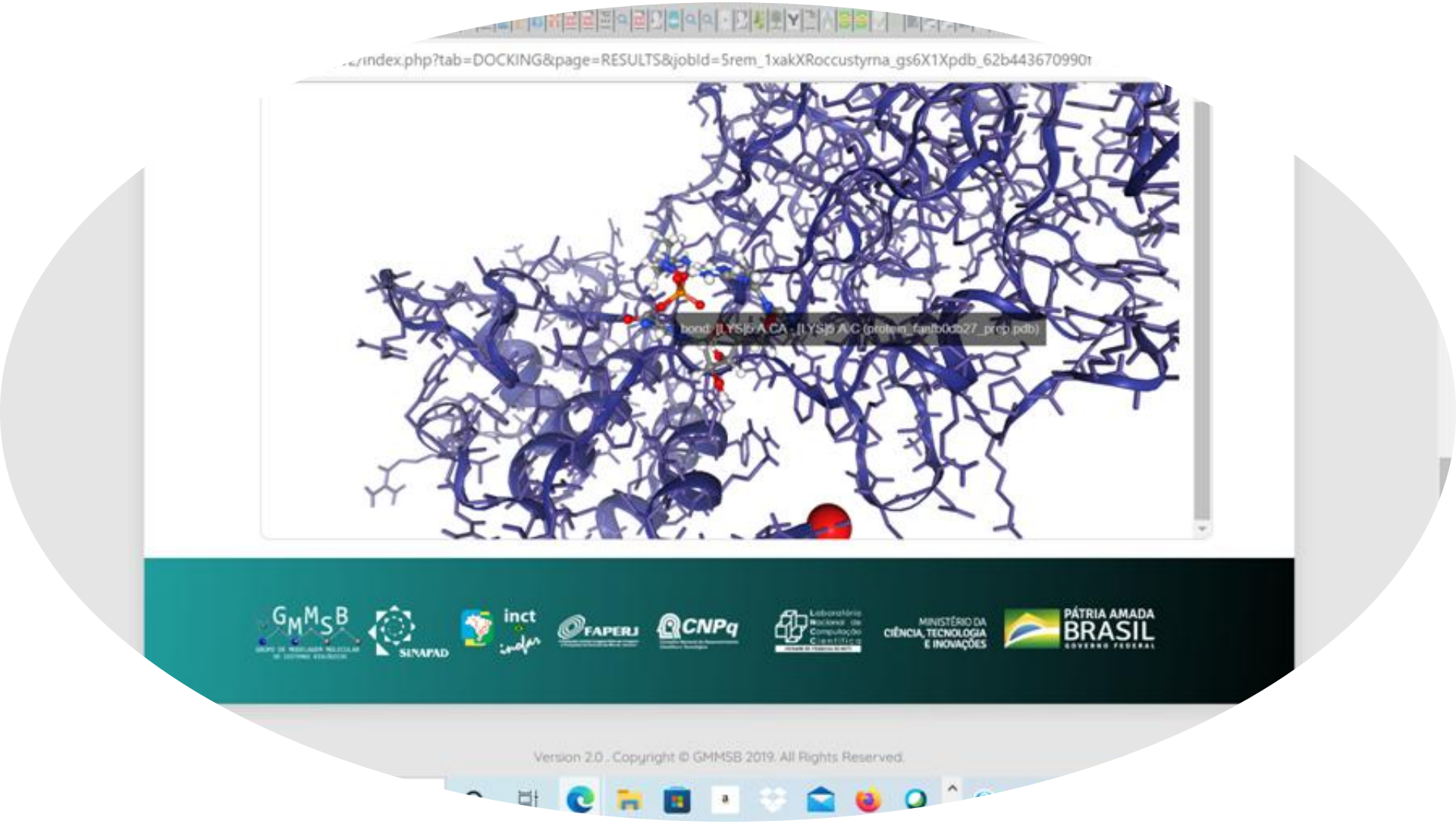
index.php?tab=DOCKING&page=RESULTS&jobId=5rem_1xakXRoccustyrna_gs6X1Xpdb_62b443670990
bond [LYS]B A CA - [LYS]B A C (protein_fanfb0db27_prep.pdb)
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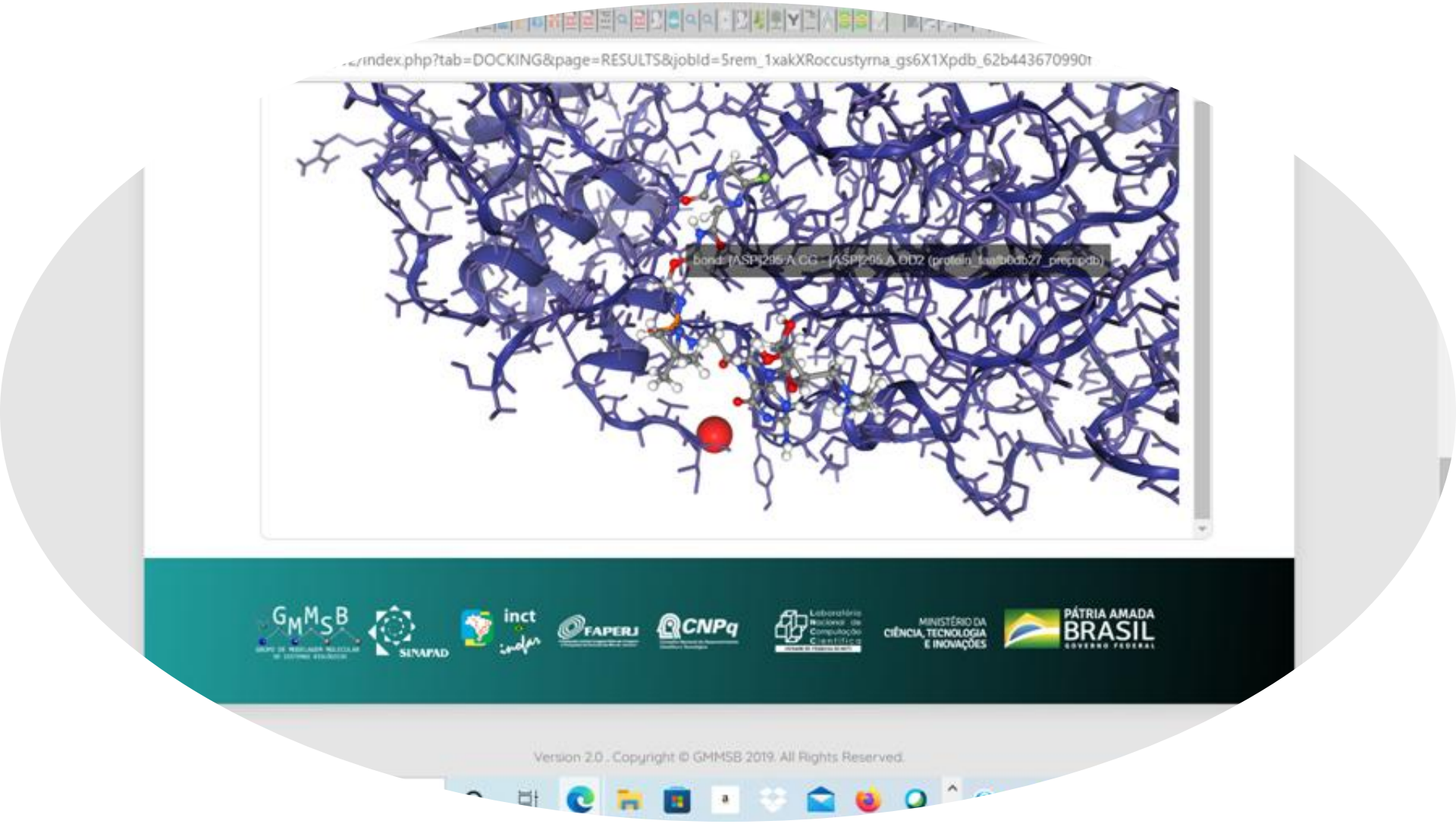

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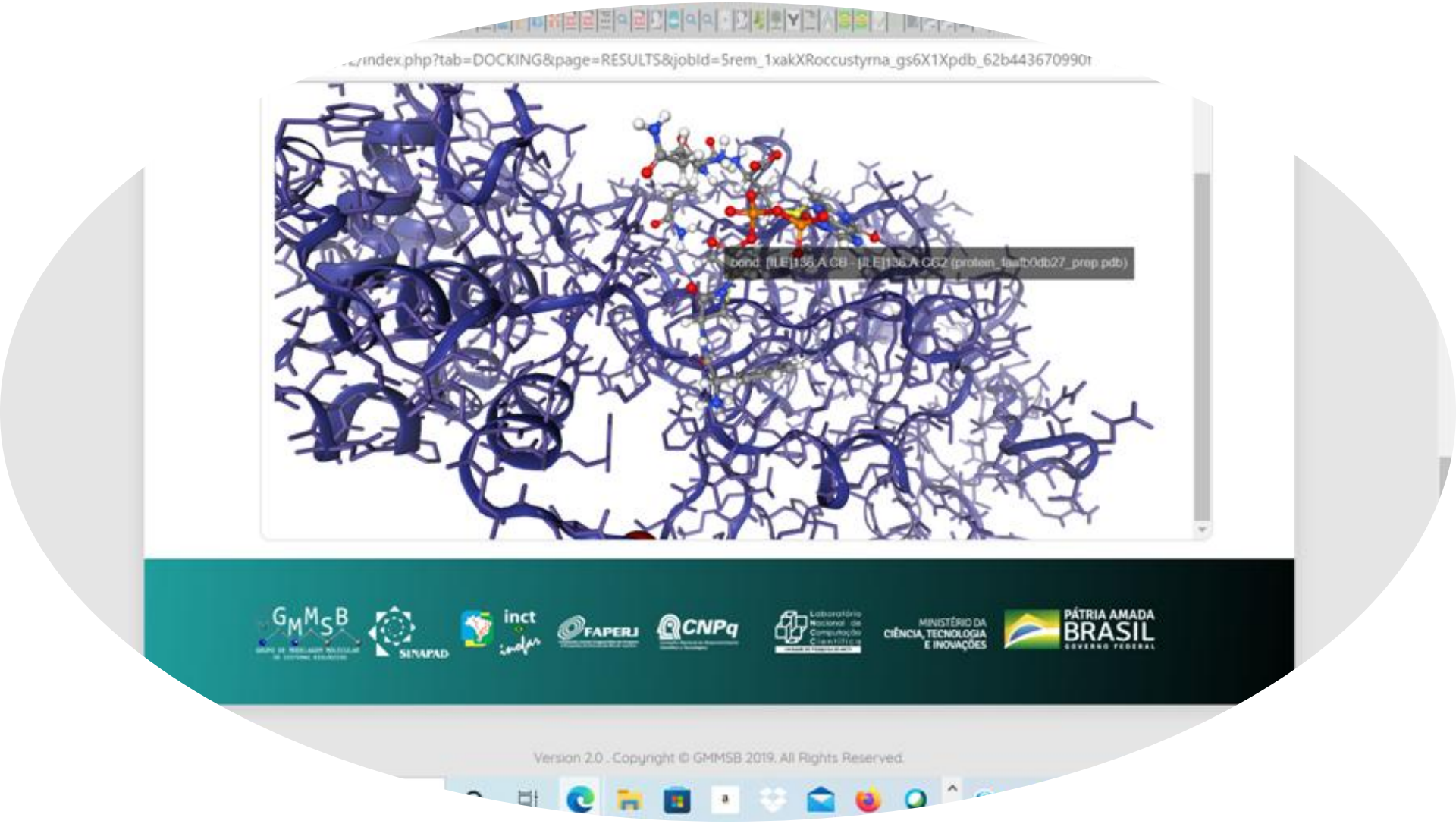
index.php?tab=DOCKING&page=RESULTS&jobId=5rem_1xakXRoccustyrna_gs6X1Xpdb_62b443670990
bond: [ILE]136.A.CB - [ILE]136.A.CG2 (protein_faafb0db27_prep.pdb)
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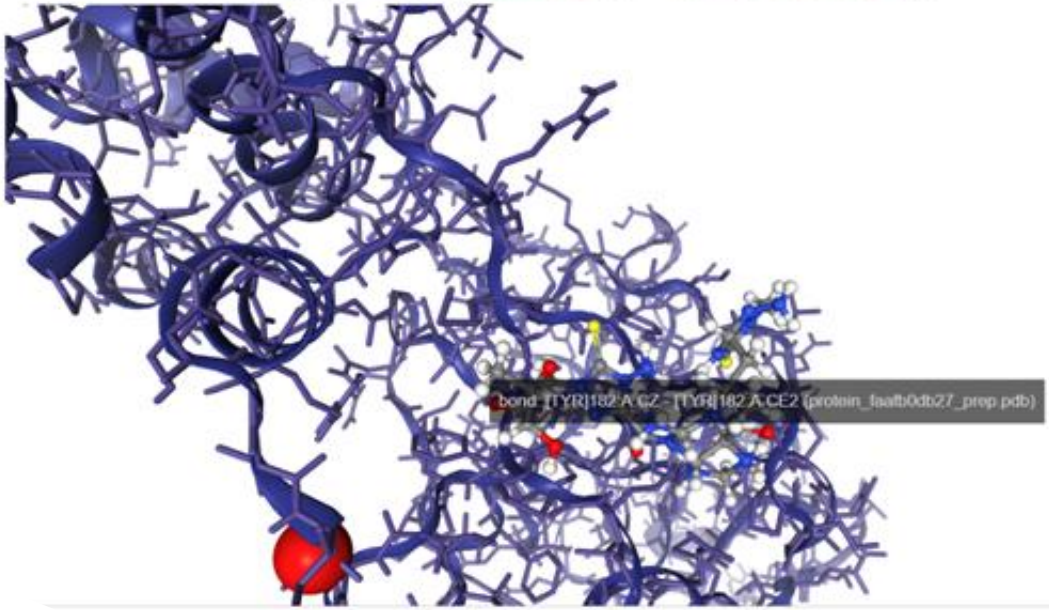
index.php?tab=DOCKING&page=RESULTS&jobId=5rem_1xakXRoccustyrna_gs6X1Xpdb_62b443670990

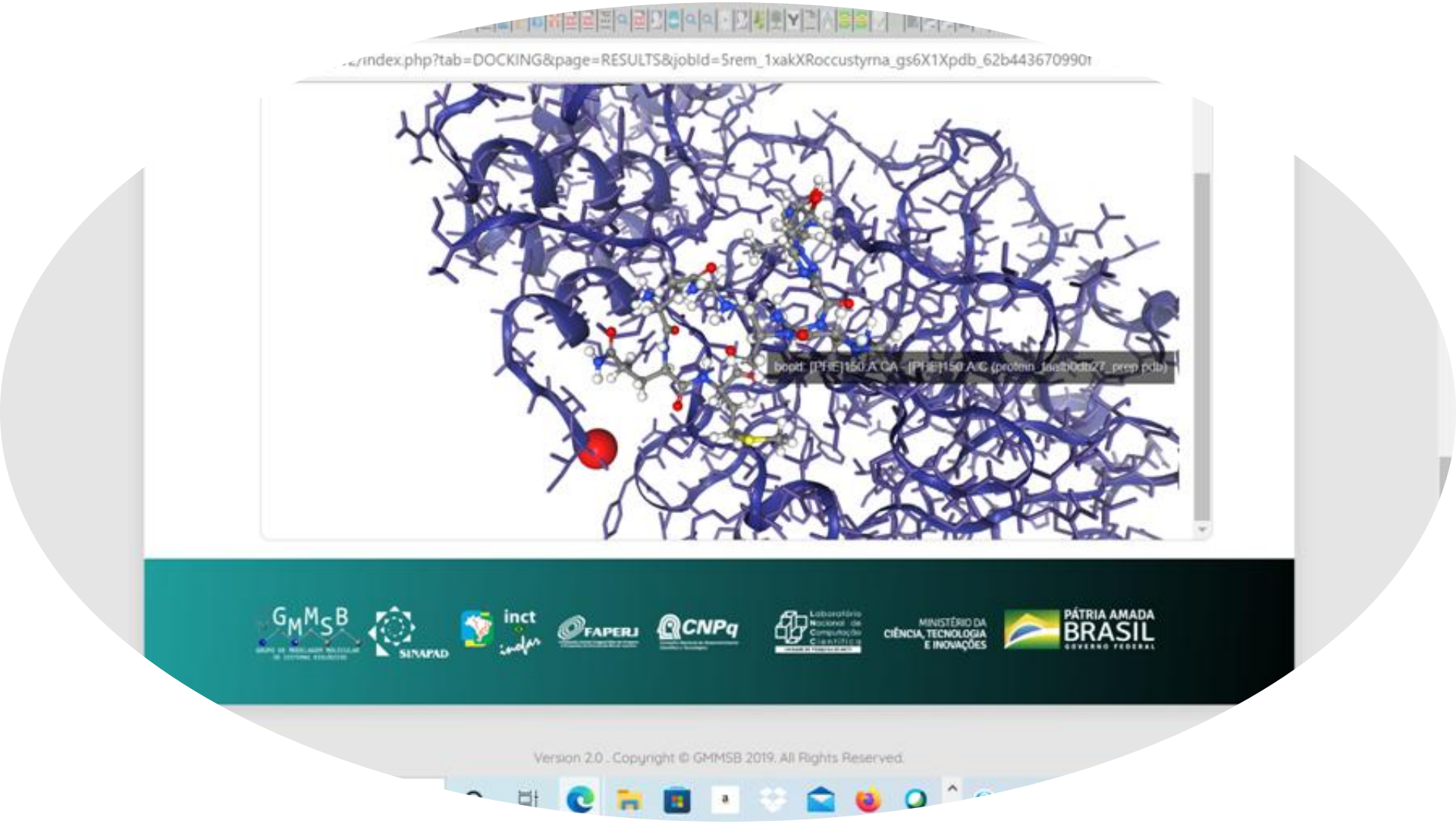
« 1 2 3 »

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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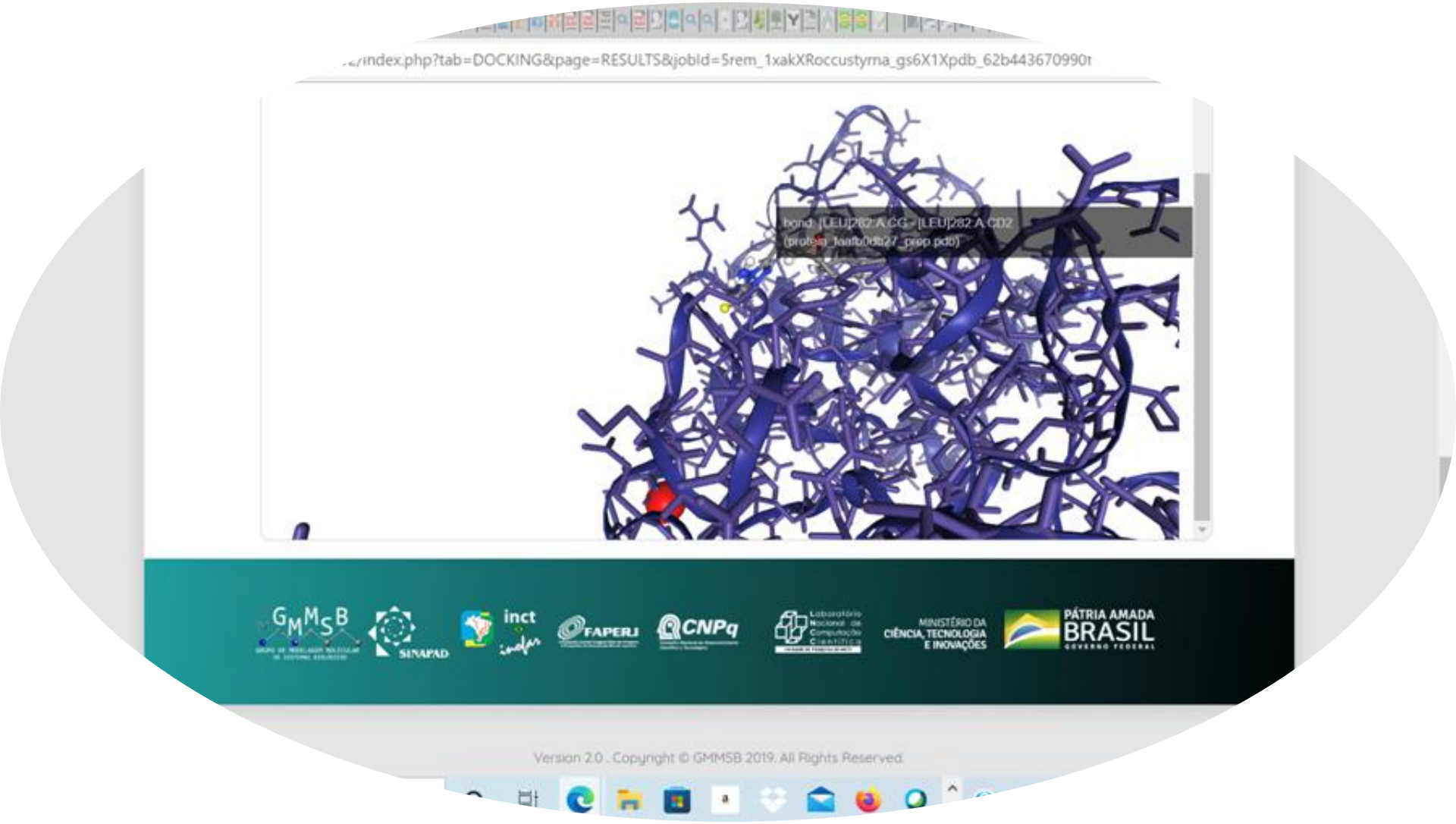
index.php?tab=DOCKING&page=RESULTS&jobId=5rem_1xakXRoccustyrna_gs6X1Xpdb_62b443670990
bond: [LEU]282:A:CG - [LEU]282:A:CD2
(protein_1aafb0db27_prep.pdb)
GMMSB
SINAPAD
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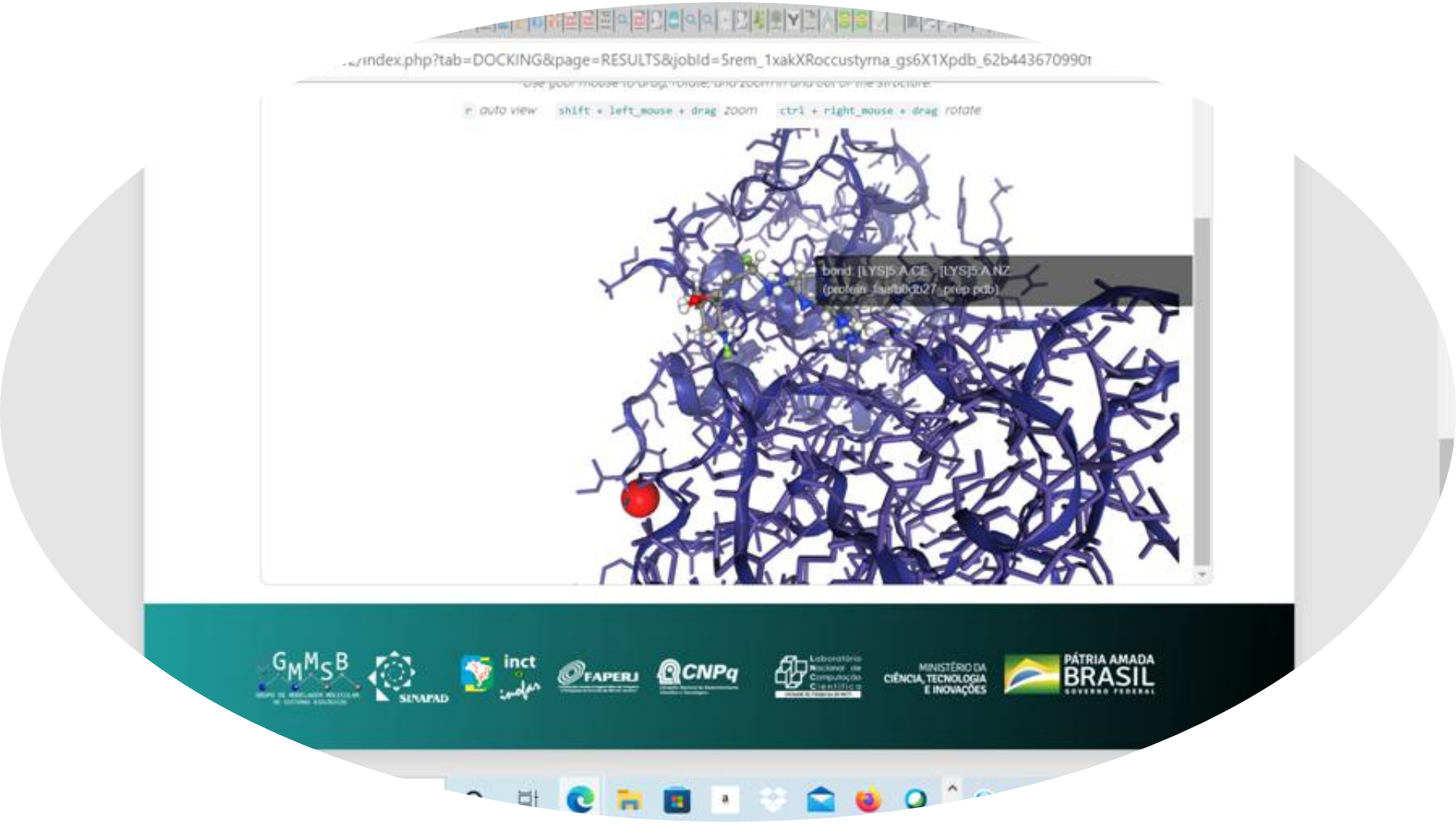
index.php?tab=DOCKING&page=RESULTS&jobId=5rem_1xakXRoccustyrna_gs6X1Xpdb_62b443670990
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [LYS]5:A.CE - [LYS]5:A.NZ
(protein_fae5b0b27_prep.pdb)
GMMSB
SENAPAD
inct
FAPERJ
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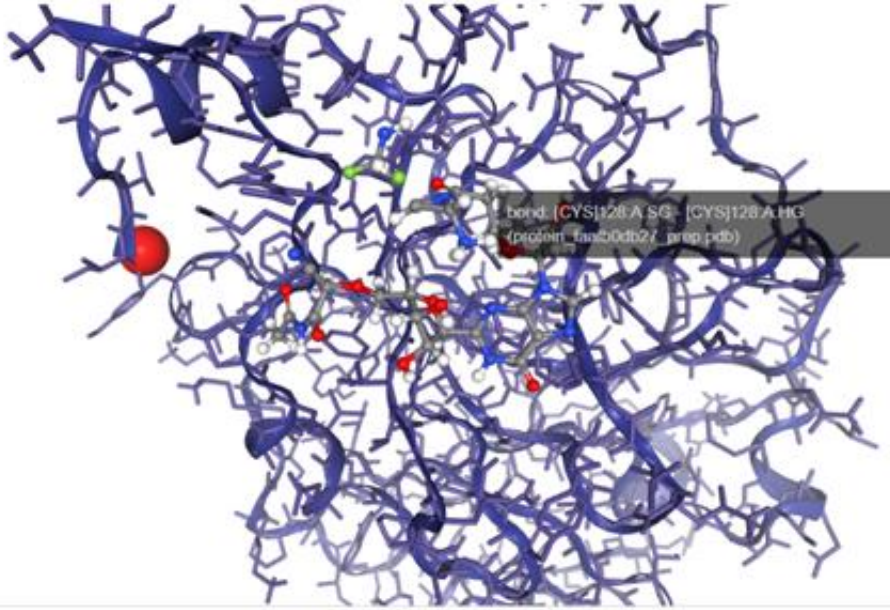
index.php?tab=DOCKING&page=RESULTS&jobId=5rem_1xakXRoccustyrna_gs6X1Xpdb_62b443670990

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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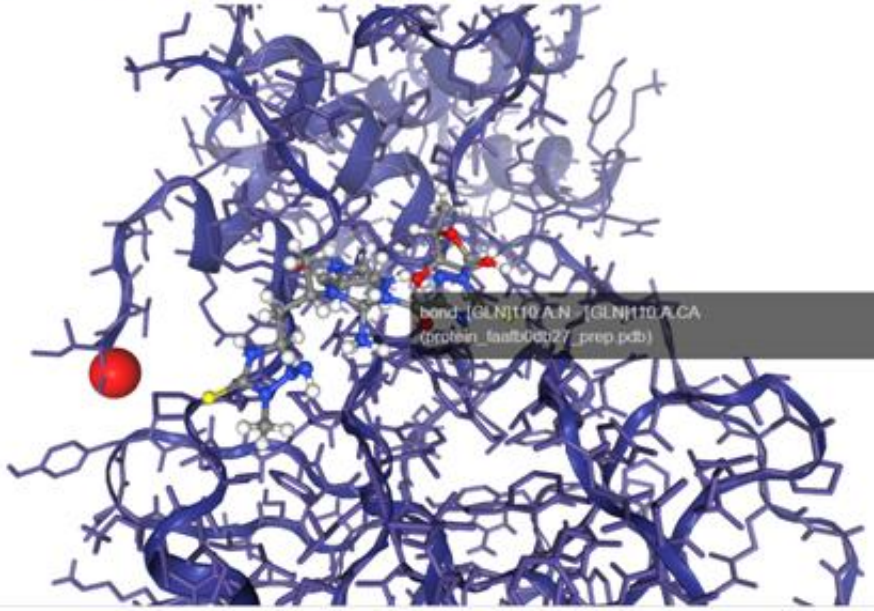
3D View

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*



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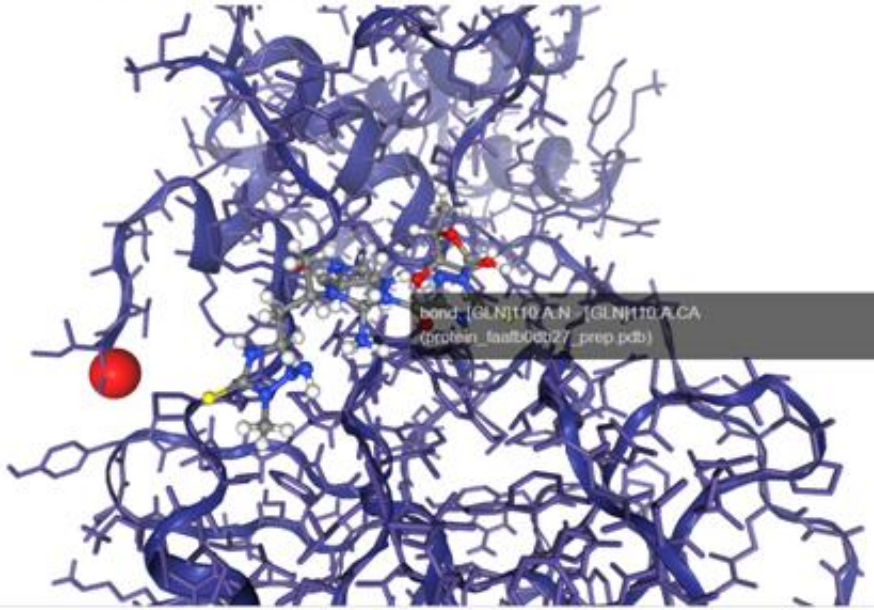
3D View

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*



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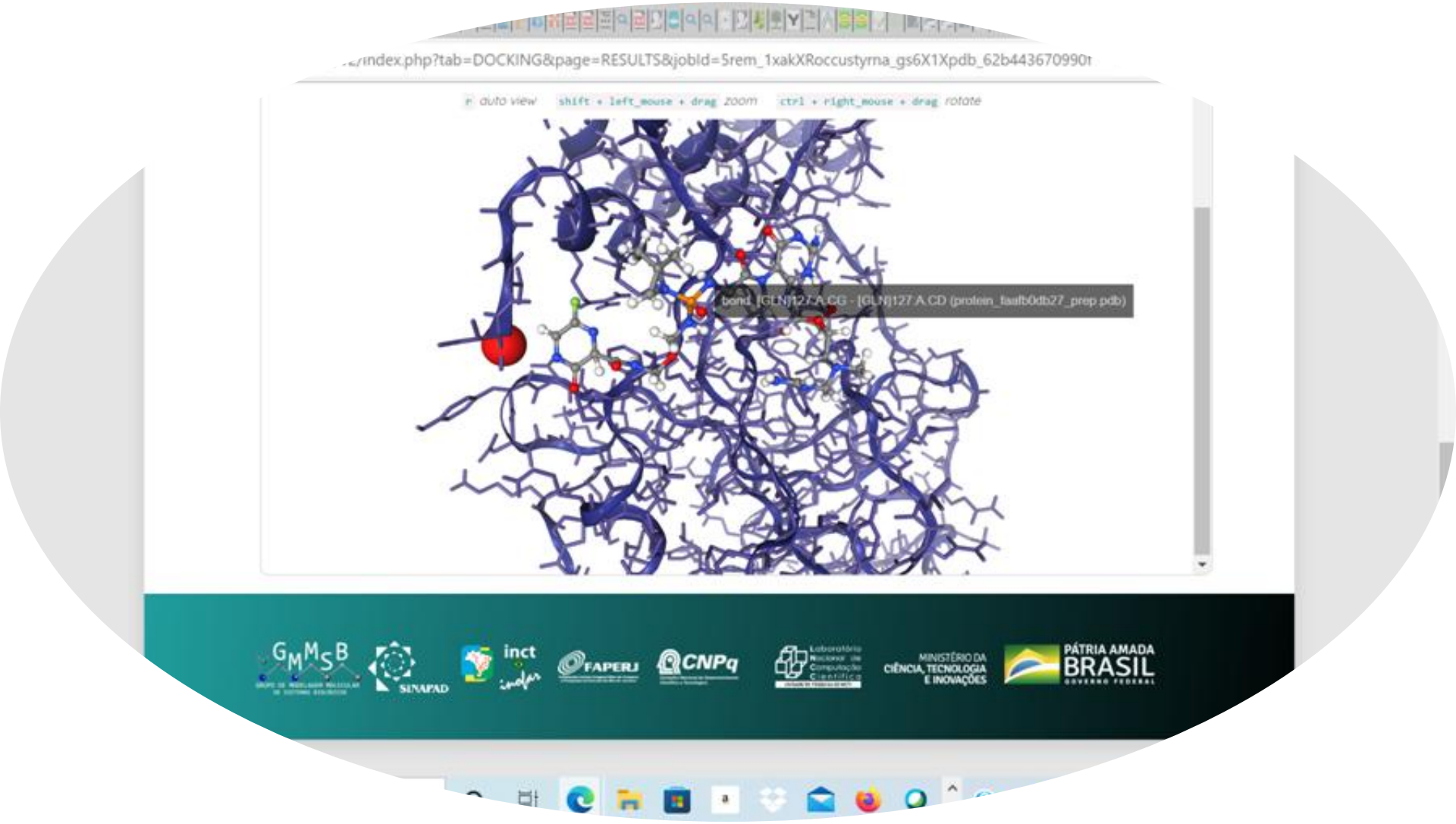
index.php?tab=DOCKING&page=RESULTS&jobId=5rem_1xakXRoccustyrna_gs6X1Xpdb_62b443670990
auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond_[GLN]127:A:CG - [GLN]127:A:CD (protein_fault0db27_prep.pdb)
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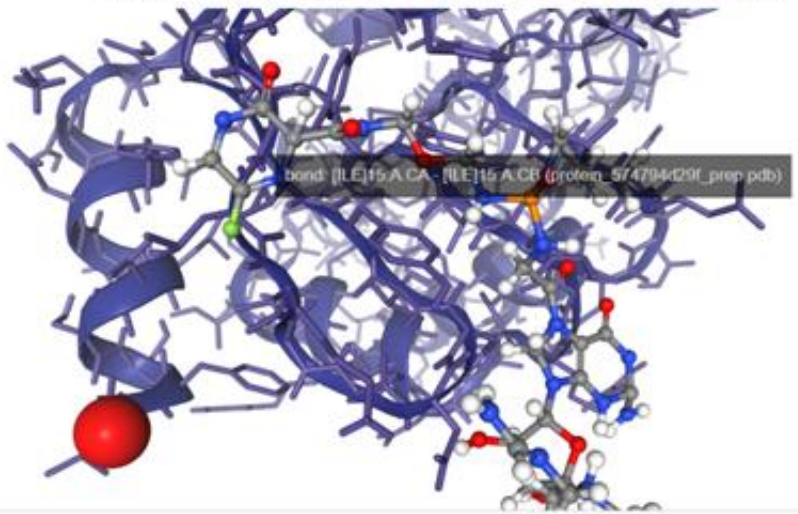
index.php?tab=DOCKING&page=RESULTS&jobId=7tx5_1xakXRoccustyrna_gs2X1Xpdb_62b435e92f4b0

r auto view shift + left_mouse + drag zoom ctrl + right_mouse + drag rotate



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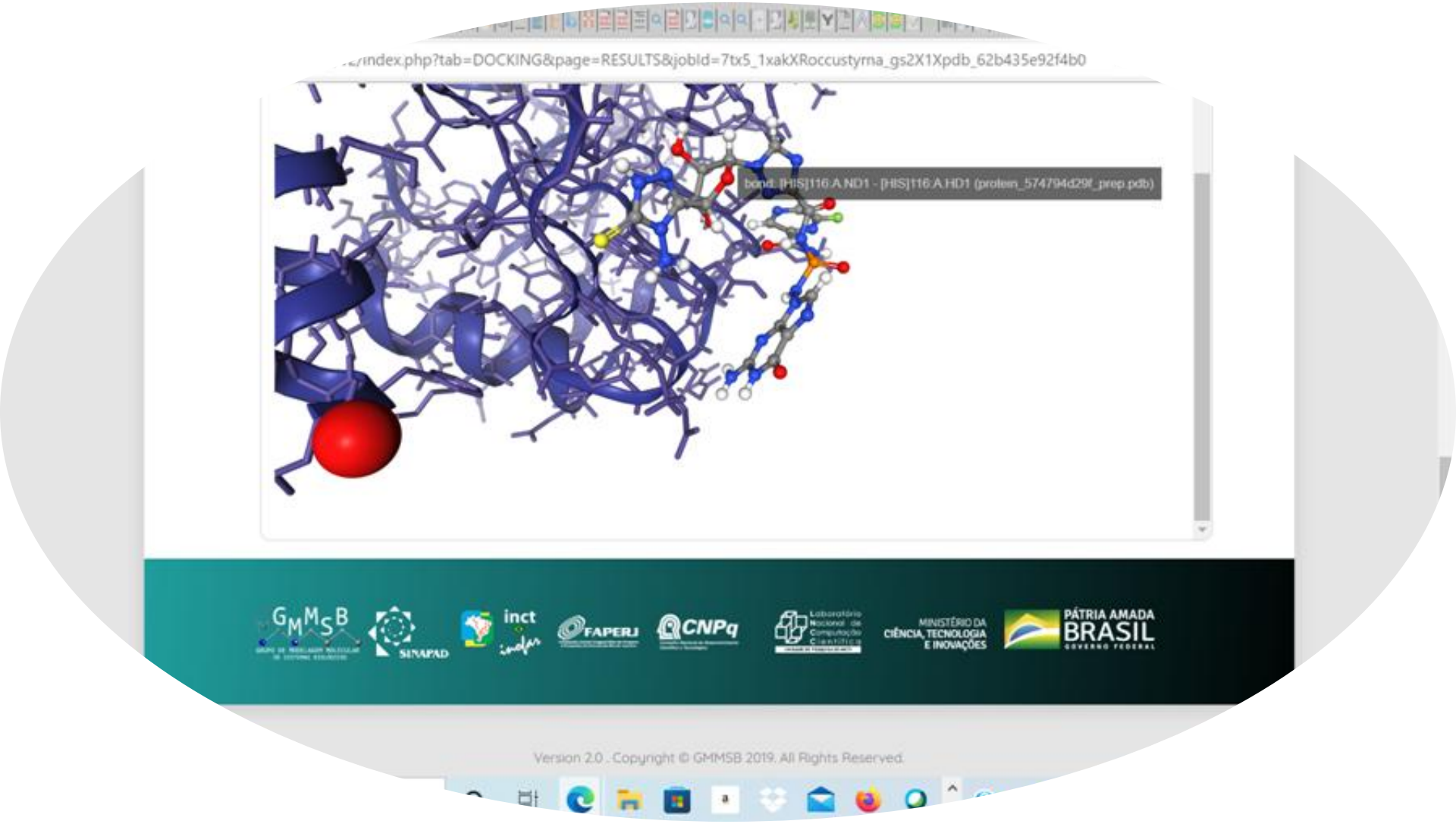
index.php?tab=DOCKING&page=RESULTS&jobId=7tx5_1xakXRoccustyrna_gs2X1Xpdb_62b435e92f4b0
bond: [HIS]116:A:ND1 - [HIS]116:A:HD1 (protein_574794d29f_prep.pdb)
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