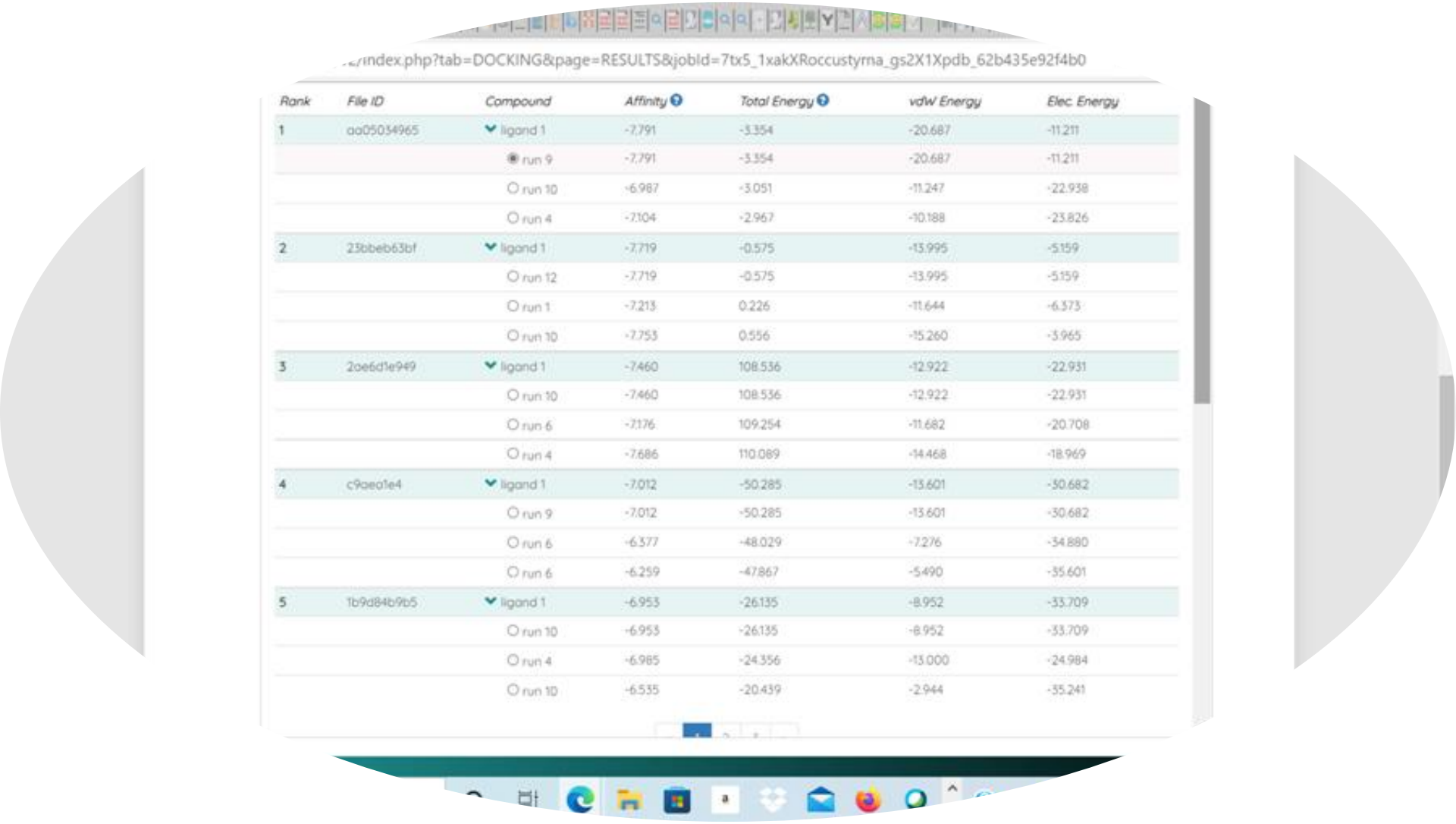
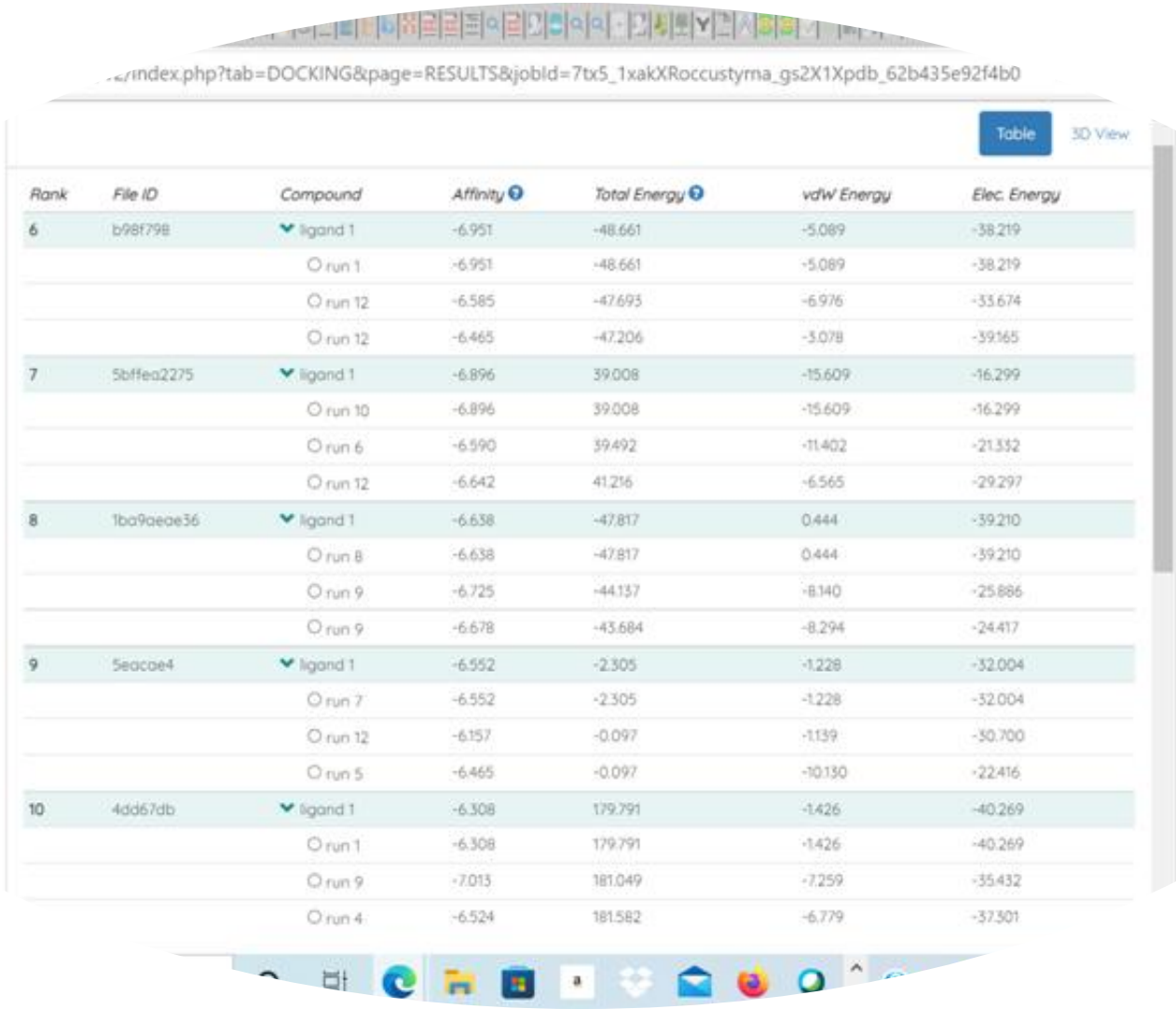


index.php?tab=DOCKING&page=RESULTS&jobId=7tx5_1xakXRoccustyrna_gs2X1Xpdb_62b435e92f4b0

Rank	File ID	Compound	Affinity	Total Energy	vdW Energy	Elec. Energy
1	aa05034965	ligand 1	-7.791	-3.354	-20.687	-11.211
		run 9	-7.791	-3.354	-20.687	-11.211
		run 10	-6.987	-3.051	-11.247	-22.938
		run 4	-7.104	-2.967	-10.188	-23.826
2	23bbeb63bf	ligand 1	-7.719	-0.575	-13.995	-5.159
		run 12	-7.719	-0.575	-13.995	-5.159
		run 1	-7.213	0.226	-11.644	-6.373
		run 10	-7.753	0.556	-15.260	-3.965
3	2ae6d1e949	ligand 1	-7.460	108.536	-12.922	-22.931
		run 10	-7.460	108.536	-12.922	-22.931
		run 6	-7.176	109.254	-11.682	-20.708
		run 4	-7.686	110.089	-14.468	-18.969
4	c9aea1e4	ligand 1	-7.012	-50.285	-13.601	-30.682
		run 9	-7.012	-50.285	-13.601	-30.682
		run 6	-6.377	-48.029	-7.276	-34.880
		run 6	-6.259	-47.867	-5.490	-35.601
5	1b9d84b9b5	ligand 1	-6.953	-26.135	-8.952	-33.709
		run 10	-6.953	-26.135	-8.952	-33.709
		run 4	-6.985	-24.356	-13.000	-24.984
		run 10	-6.535	-20.439	-2.944	-35.241



Rank	File ID	Compound	Affinity	Total Energy	vdW Energy	Elec. Energy
6	b98f798	ligand 1	-6.951	-48.661	-5.089	-38.219
		run 1	-6.951	-48.661	-5.089	-38.219
		run 12	-6.585	-47.693	-6.976	-33.674
		run 12	-6.465	-47.206	-3.078	-39.165
7	5bffea2275	ligand 1	-6.896	39.008	-15.609	-16.299
		run 10	-6.896	39.008	-15.609	-16.299
		run 6	-6.590	39.492	-11.402	-21.332
		run 12	-6.642	41.216	-6.565	-29.297
8	1ba9aeae36	ligand 1	-6.638	-47.817	0.444	-39.210
		run 8	-6.638	-47.817	0.444	-39.210
		run 9	-6.725	-44.137	-8.140	-25.886
		run 9	-6.678	-43.684	-8.294	-24.417
9	5eacae4	ligand 1	-6.552	-2.305	-1.228	-32.004
		run 7	-6.552	-2.305	-1.228	-32.004
		run 12	-6.157	-0.097	-1.139	-30.700
		run 5	-6.465	-0.097	-10.130	-22.416
10	4dd67db	ligand 1	-6.308	179.791	-1.426	-40.269
		run 1	-6.308	179.791	-1.426	-40.269
		run 9	-7.013	181.049	-7.259	-35.432
		run 4	-6.524	181.582	-6.779	-37.301

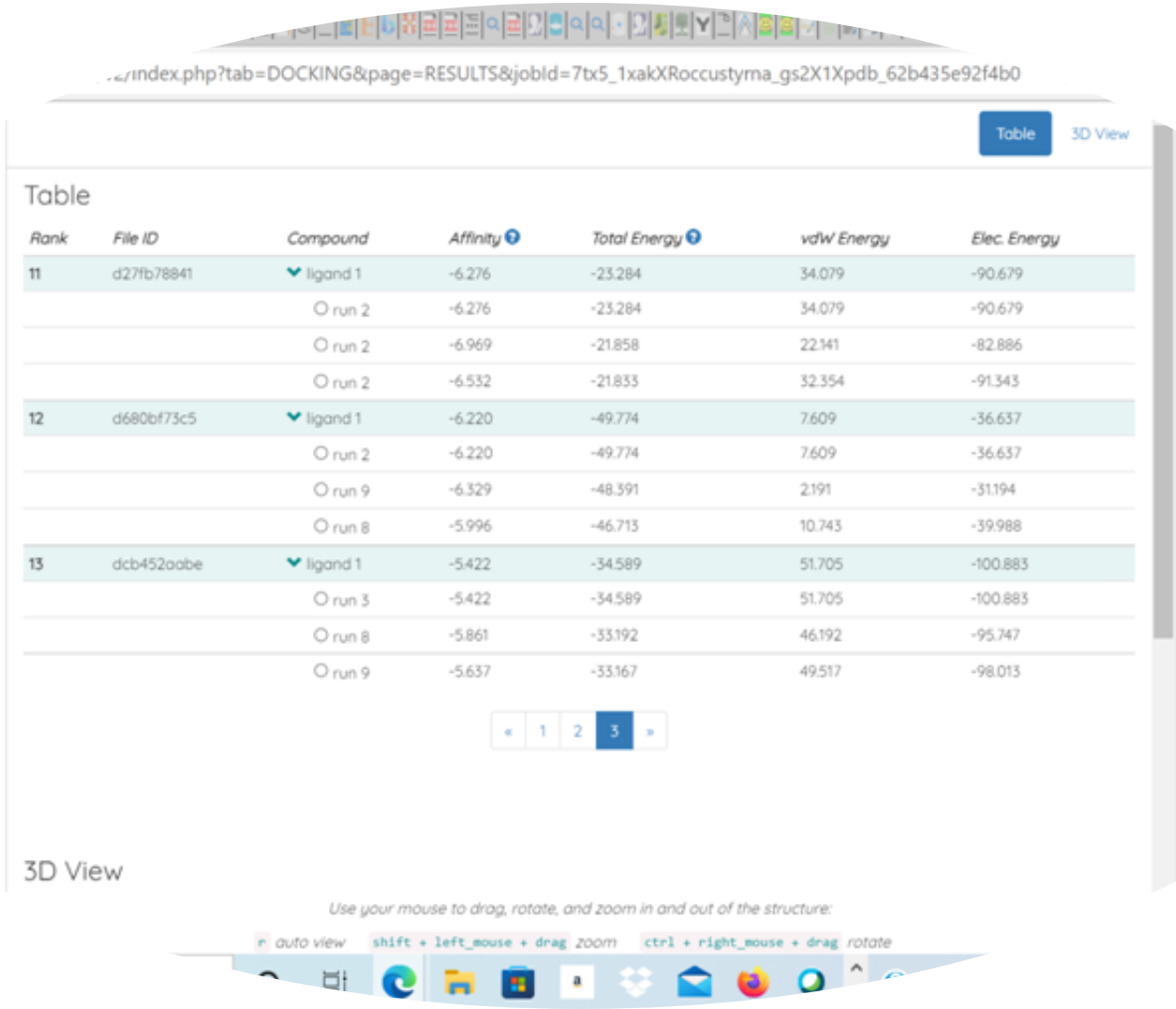

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Table
3D View
Table
Rank File ID Compound Affinity Total Energy vdW Energy Elec. Energy
11 d27fb78841 ligand 1 -6.276 -23.284 34.079 -90.679
run 2 -6.276 -23.284 34.079 -90.679
run 2 -6.969 -21.858 22.141 -82.886
run 2 -6.532 -21.833 32.354 -91.343
12 d680bf73c5 ligand 1 -6.220 -49.774 7.609 -36.637
run 2 -6.220 -49.774 7.609 -36.637
run 9 -6.329 -48.391 2.191 -31.194
run 8 -5.996 -46.713 10.743 -39.988
13 dcb452aabe ligand 1 -5.422 -34.589 51.705 -100.883
run 3 -5.422 -34.589 51.705 -100.883
run 8 -5.861 -33.192 46.192 -95.747
run 9 -5.637 -33.167 49.517 -98.013
« 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

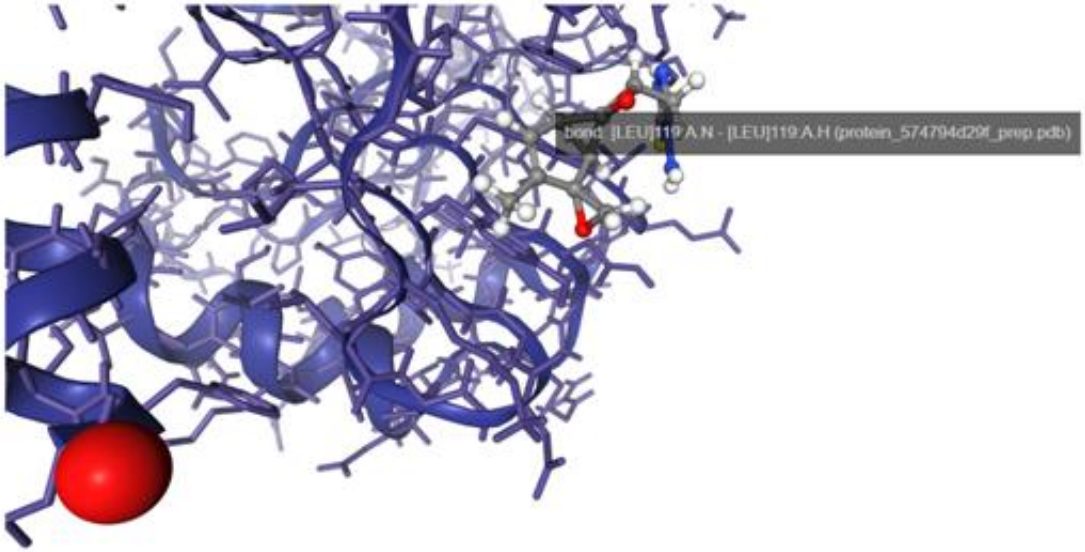
index.php?tab=DOCKING&page=RESULTS&jobId=7tx5_1xakXRoccustyrna_gs2X1Xpdb_62b435e92f4b0

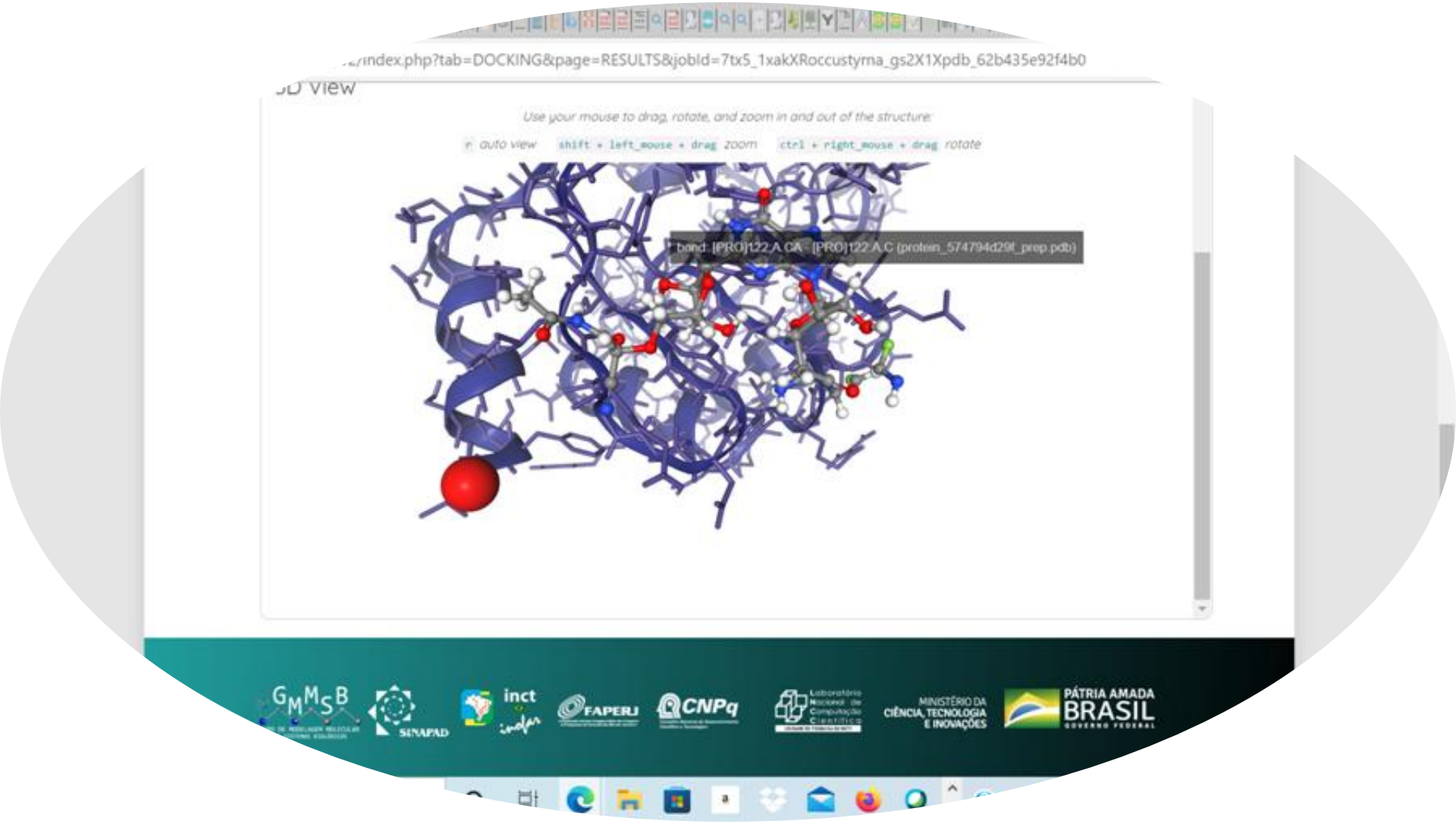
« 1 2 3 »

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=7tx5_1xakXRoccustyrna_gs2X1Xpdb_62b435e92f4b0
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
band: [PRO]122:A.CA - [PRO]122:A.C (protein_574794d29f_prep.pdb)
GMMSB
SENAPAD
inct
FAPERJ
CNPq
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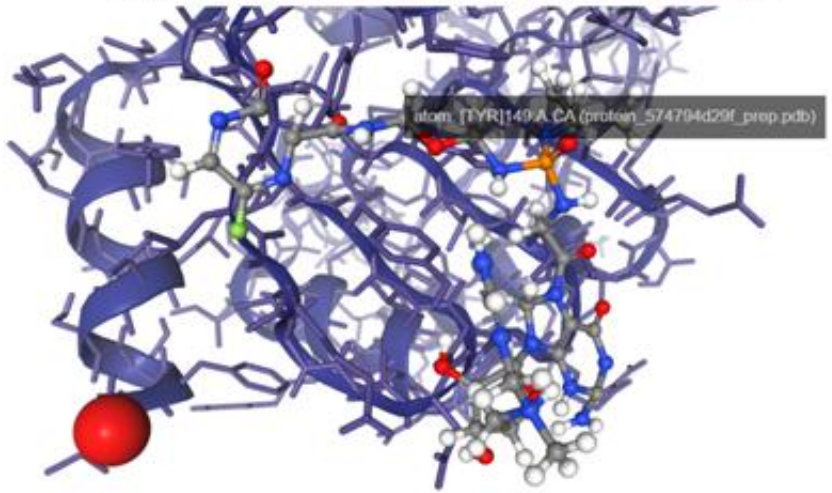
index.php?tab=DOCKING&page=RESULTS&jobId=7tx5_1xakXRoccustyrna_gs2X1Xpdb_62b435e92f4b0

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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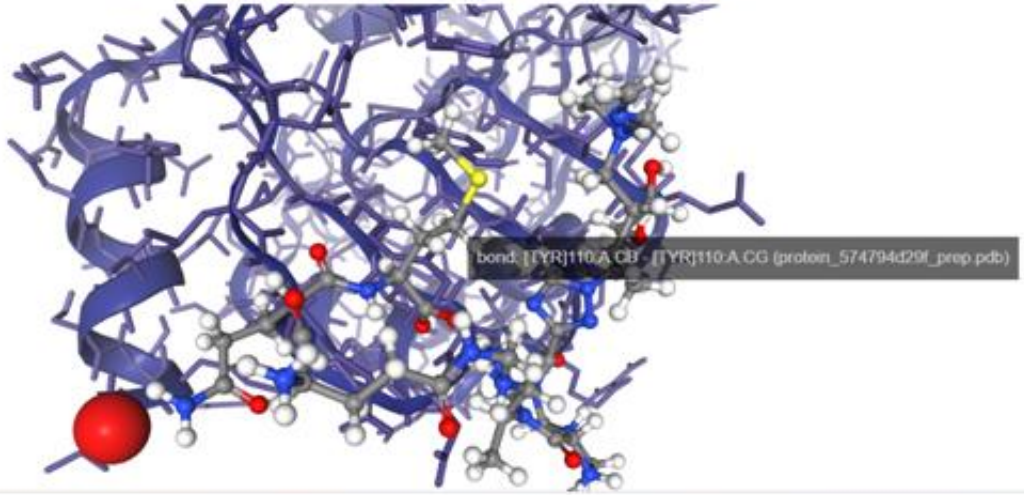
Use your mouse to drag, rotate, and zoom in and out of the structure.

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



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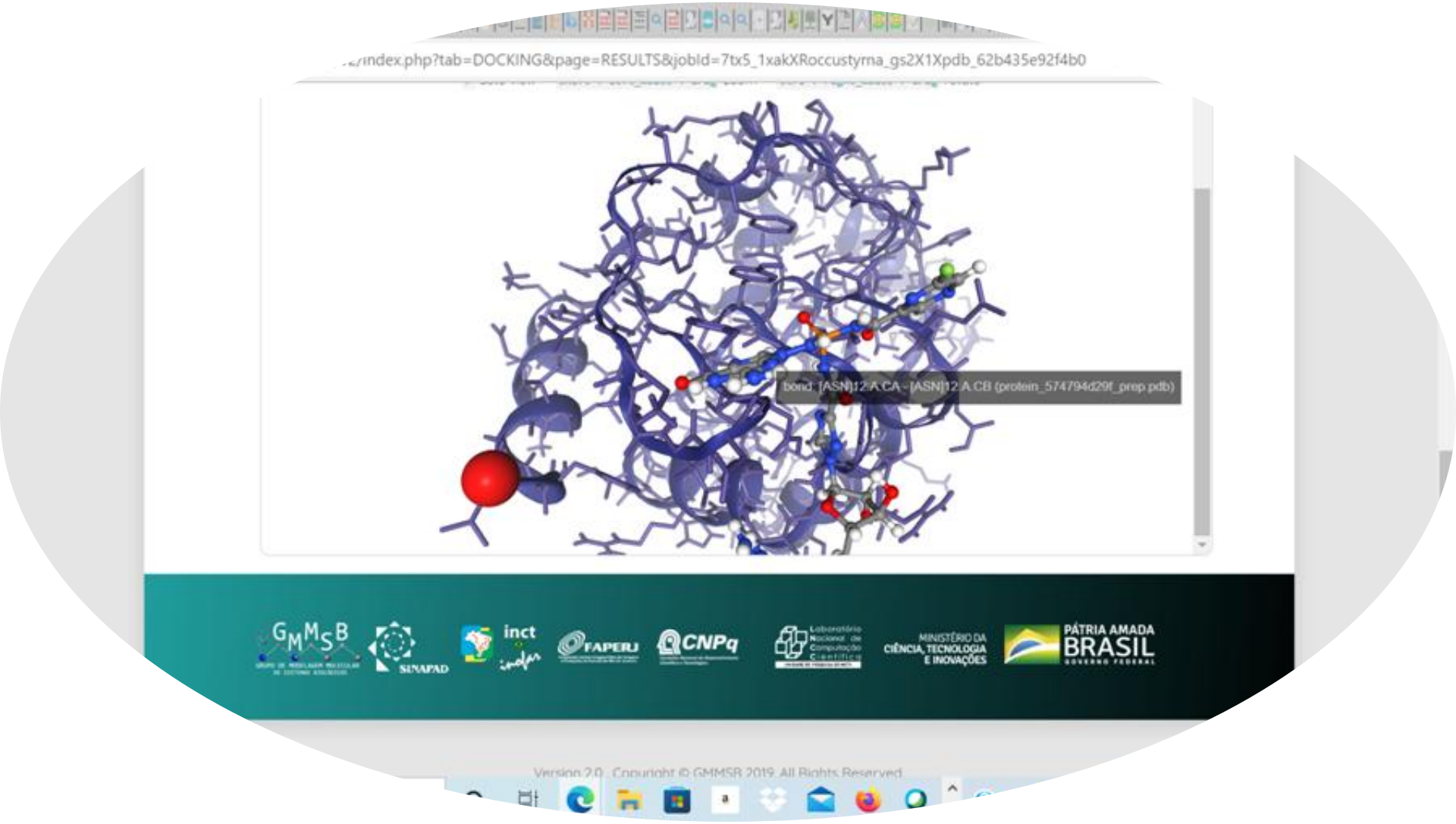
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bond: [ASN]12:A:CA - [ASN]12:A:CB (protein_574794d29f_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
Laboratório Nacional de Computação Científica
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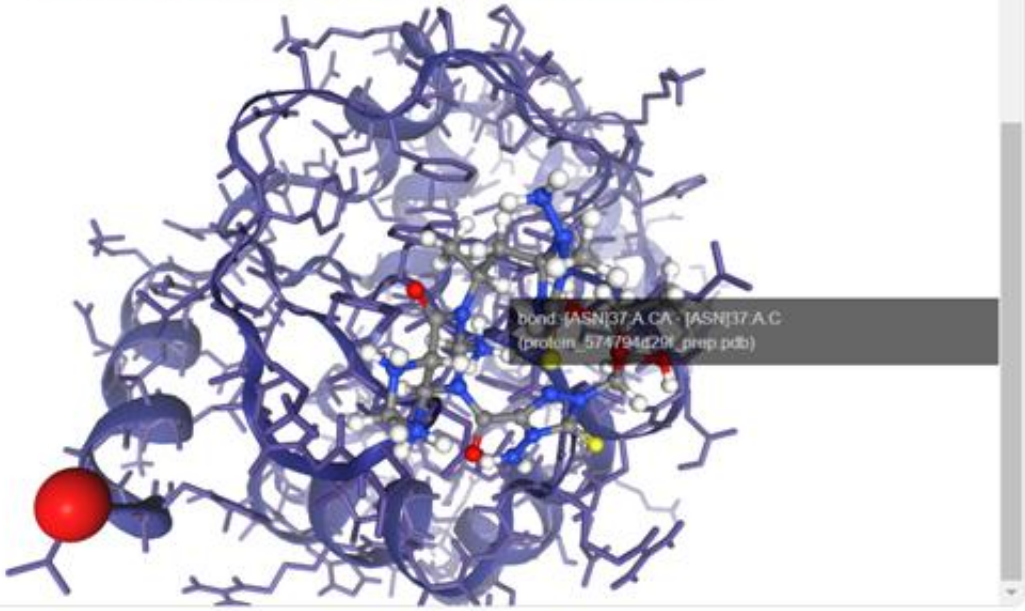
index.php?tab=DOCKING&page=RESULTS&jobId=7tx5_1xakXRoccustyrna_gs2X1Xpdb_62b435e92f4b0

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*



inct
FAPERJ
CNPq
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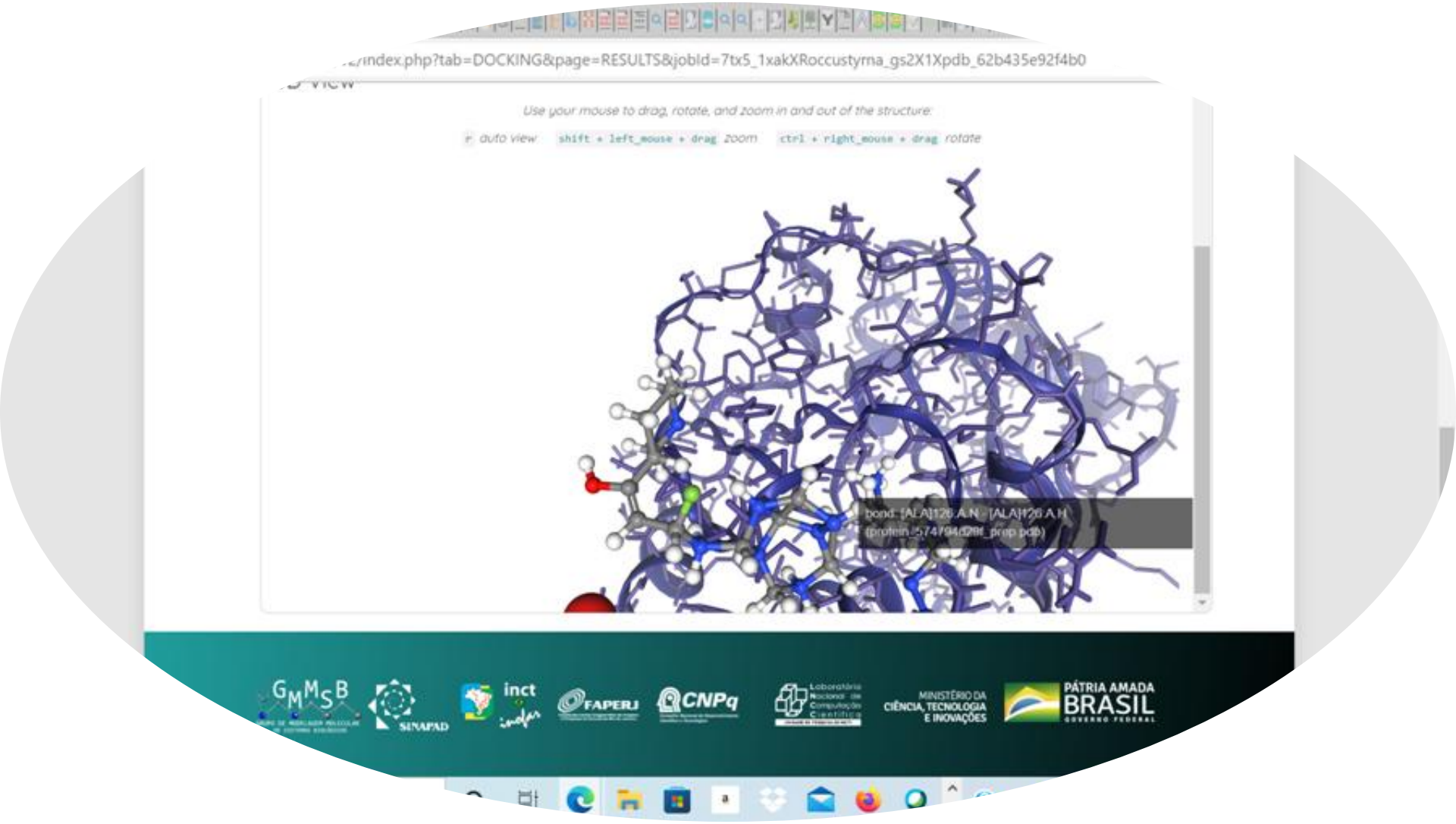
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Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [ALA]126.A.N - [ALA]126.A.H
(protein_574794d2ff_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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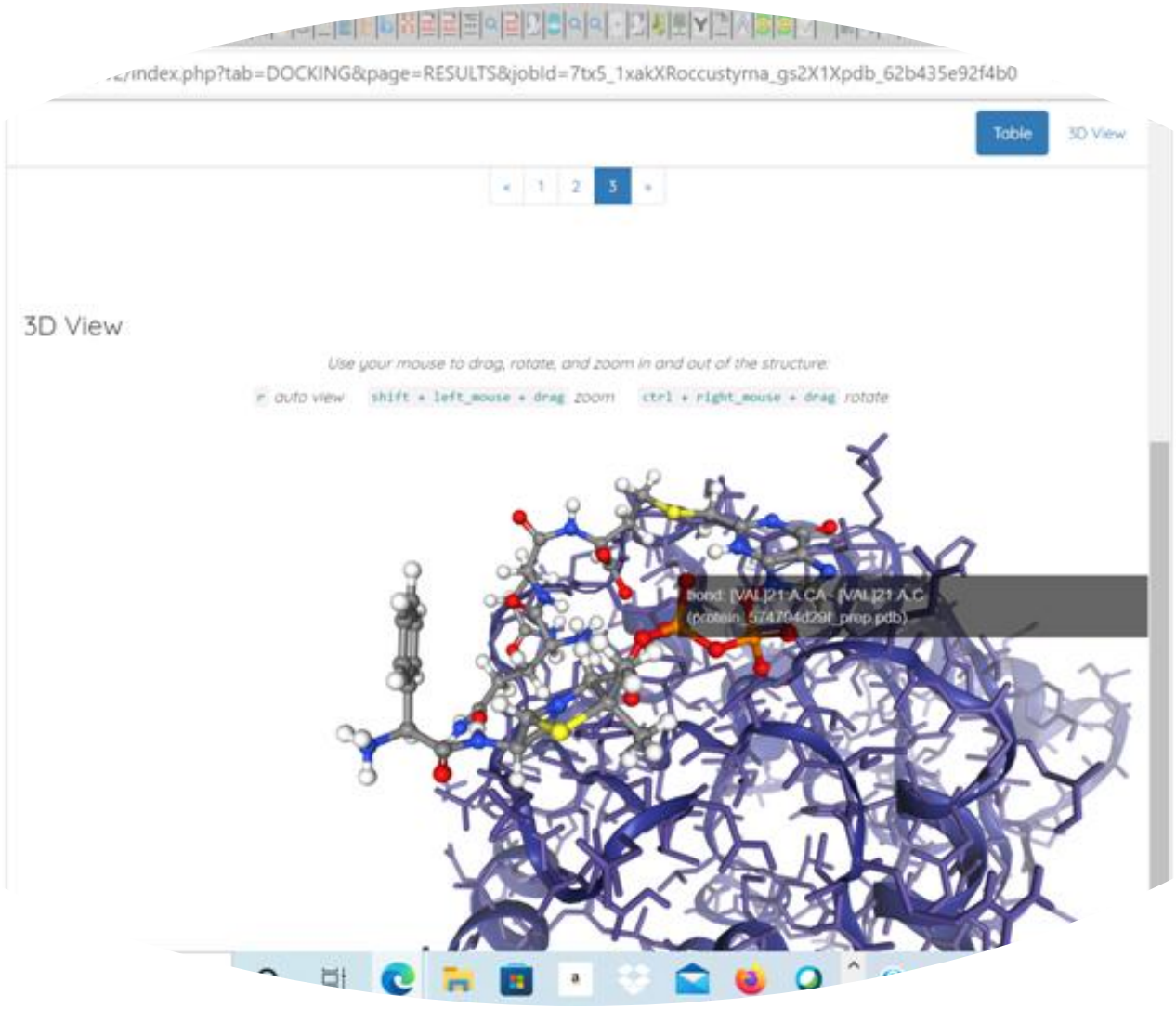
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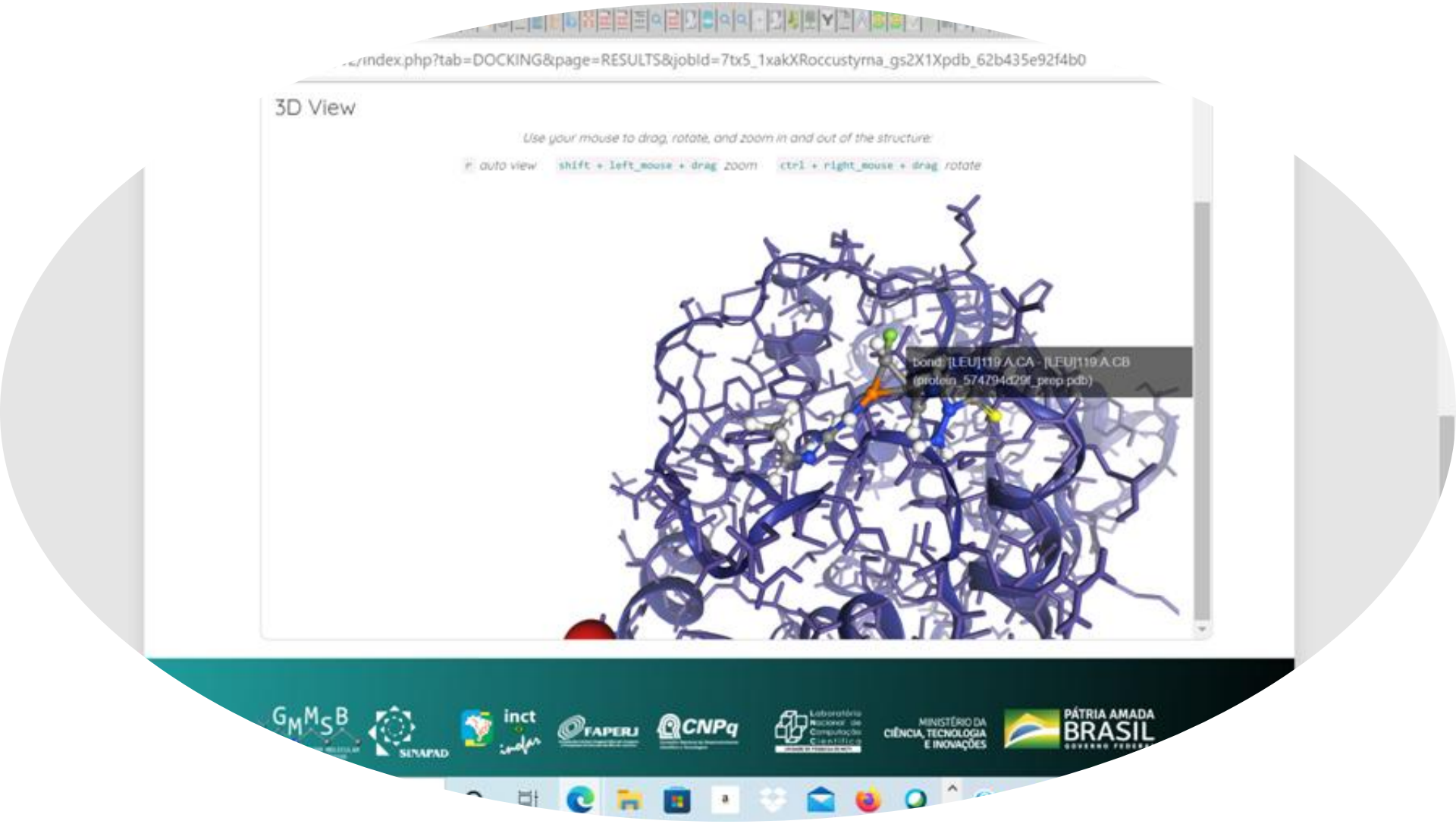
Table
3D View
« 1 2 3 »
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
Bond: [VAL]21:A.CA - [VAL]21:A.C
(protein_574704d29f_prep.pdb)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3D View
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 [LEU]119:A.CA - [LEU]119:A.CB
(protein_5747f94d29f_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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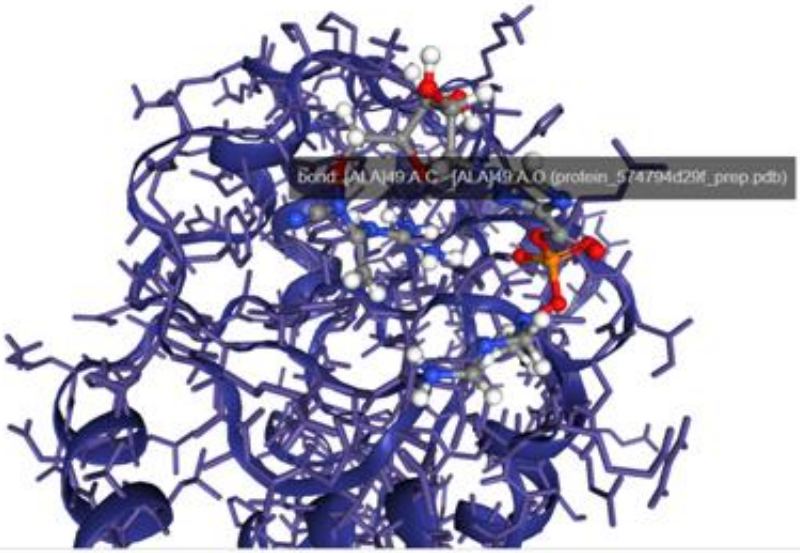

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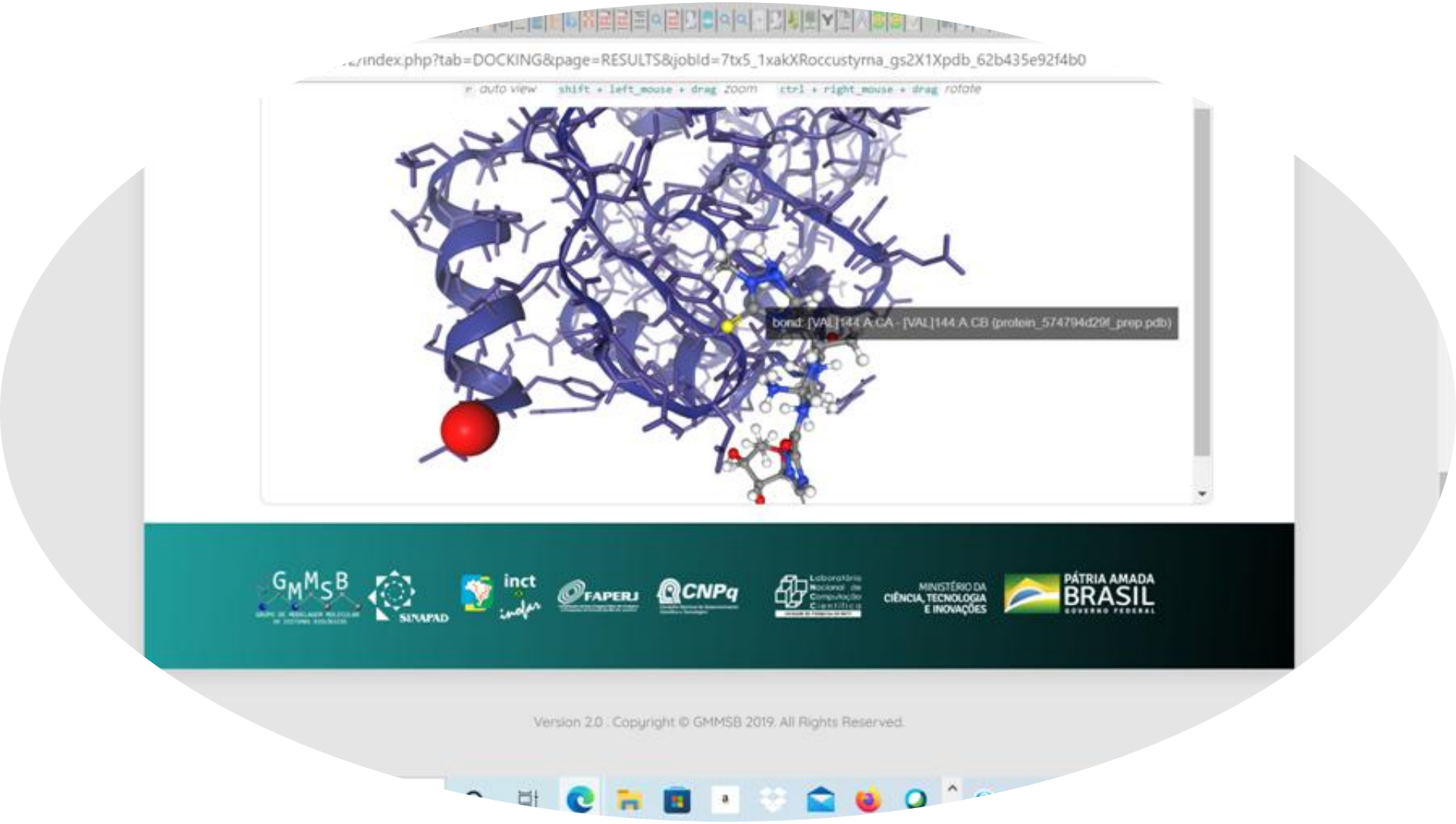
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r auto view shift + left_mouse + drag zoom ctrl + right_mouse + drag rotate
bond: [VAL]144 A.CA - [VAL]144 A.CB (protein_574794d29ff_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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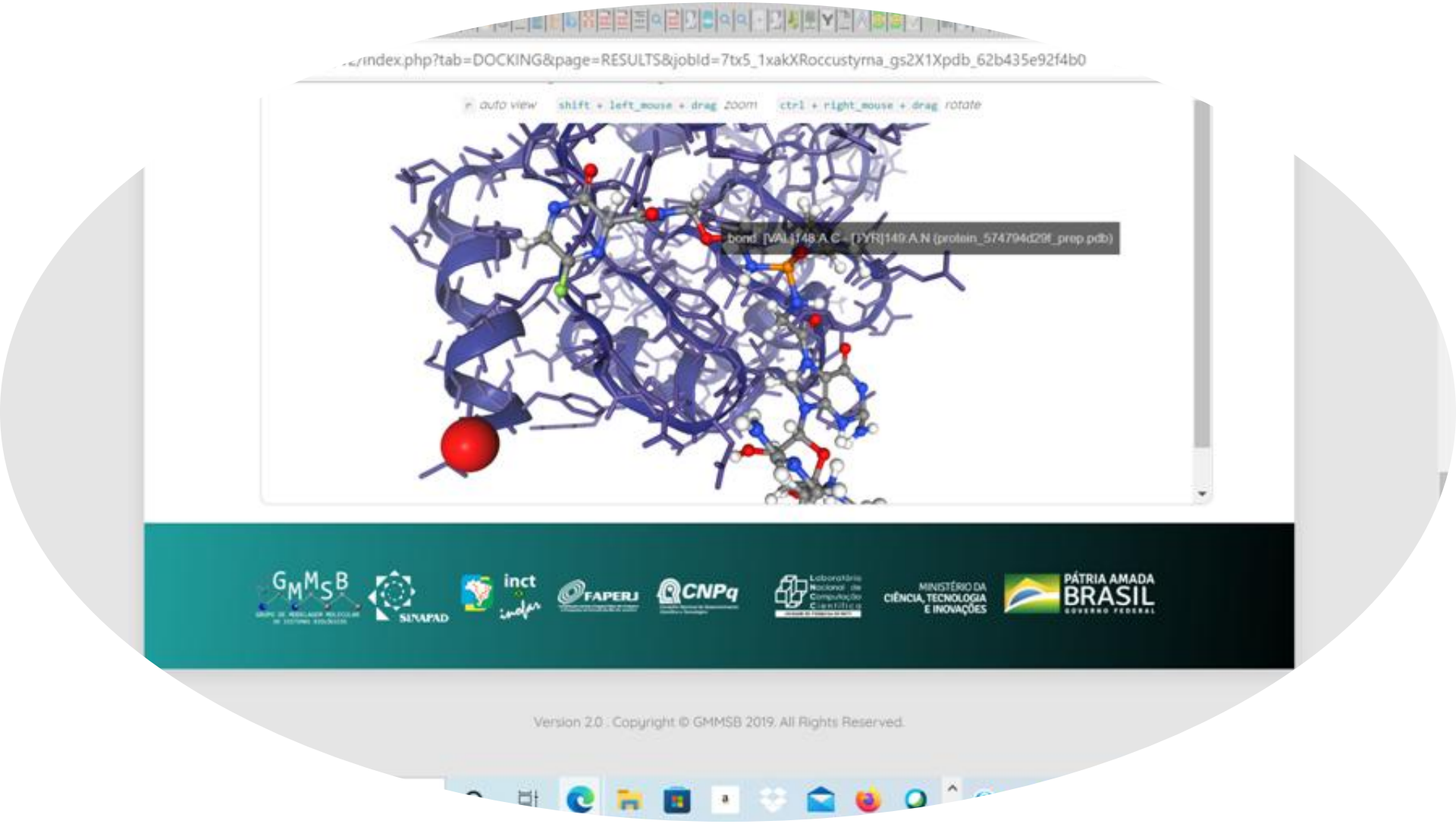
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auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond [VAL:148:A:C - TYR:149:A:N (protein_574794d29f_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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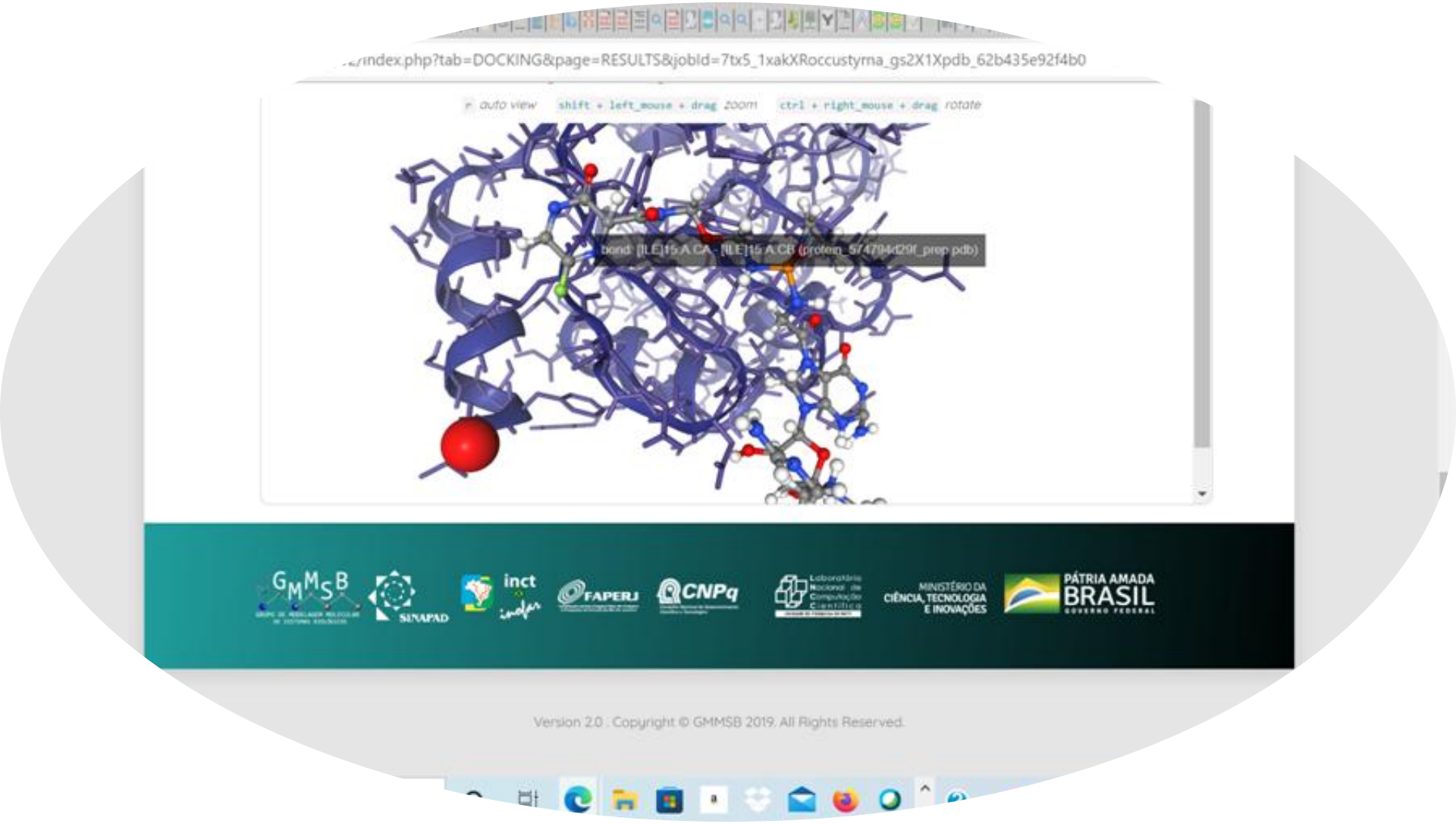
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shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [ILE]15:A:CA - [ILE]15:A:CB (protein_5747944d29f_prep.pdb)
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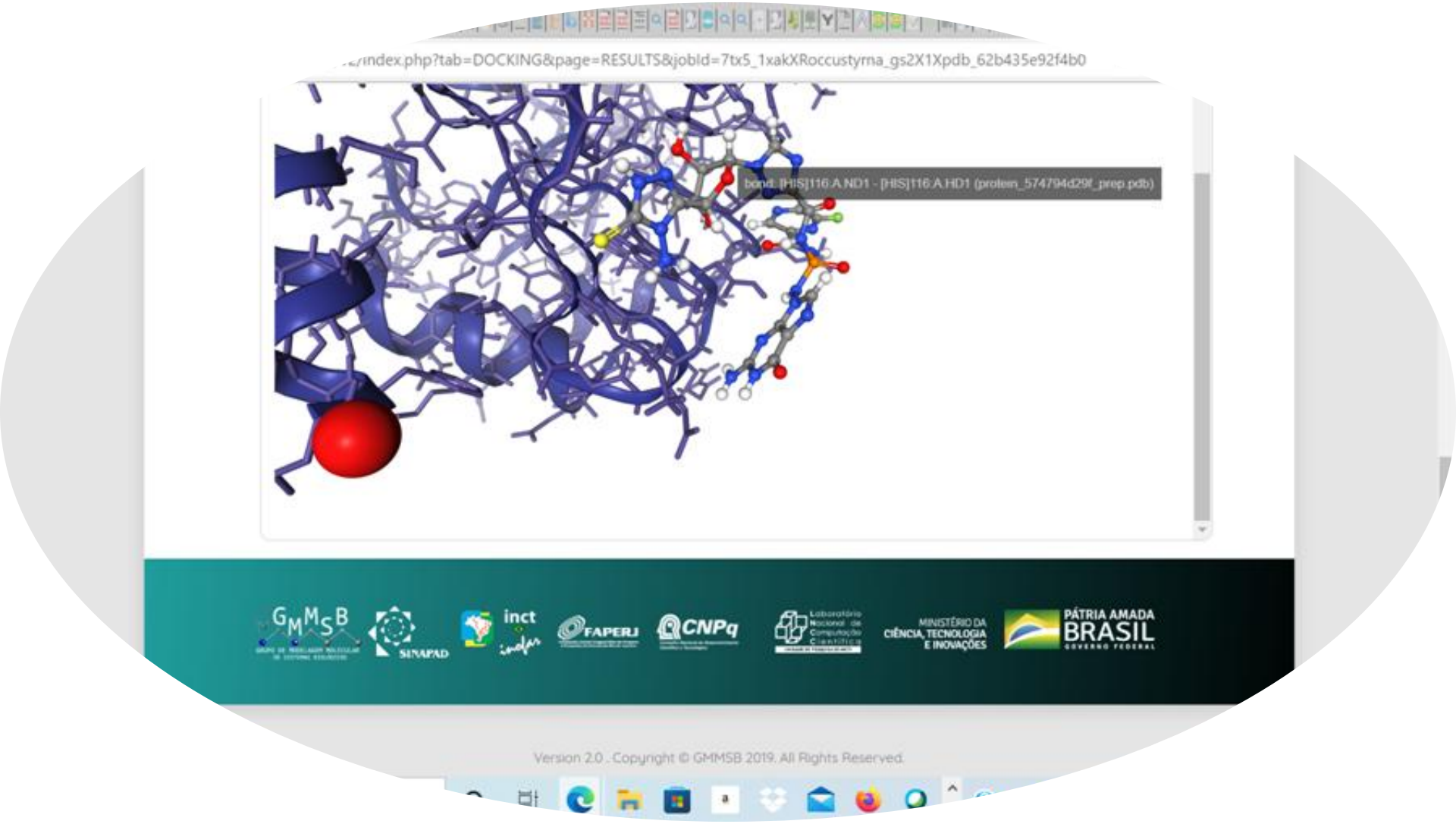
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