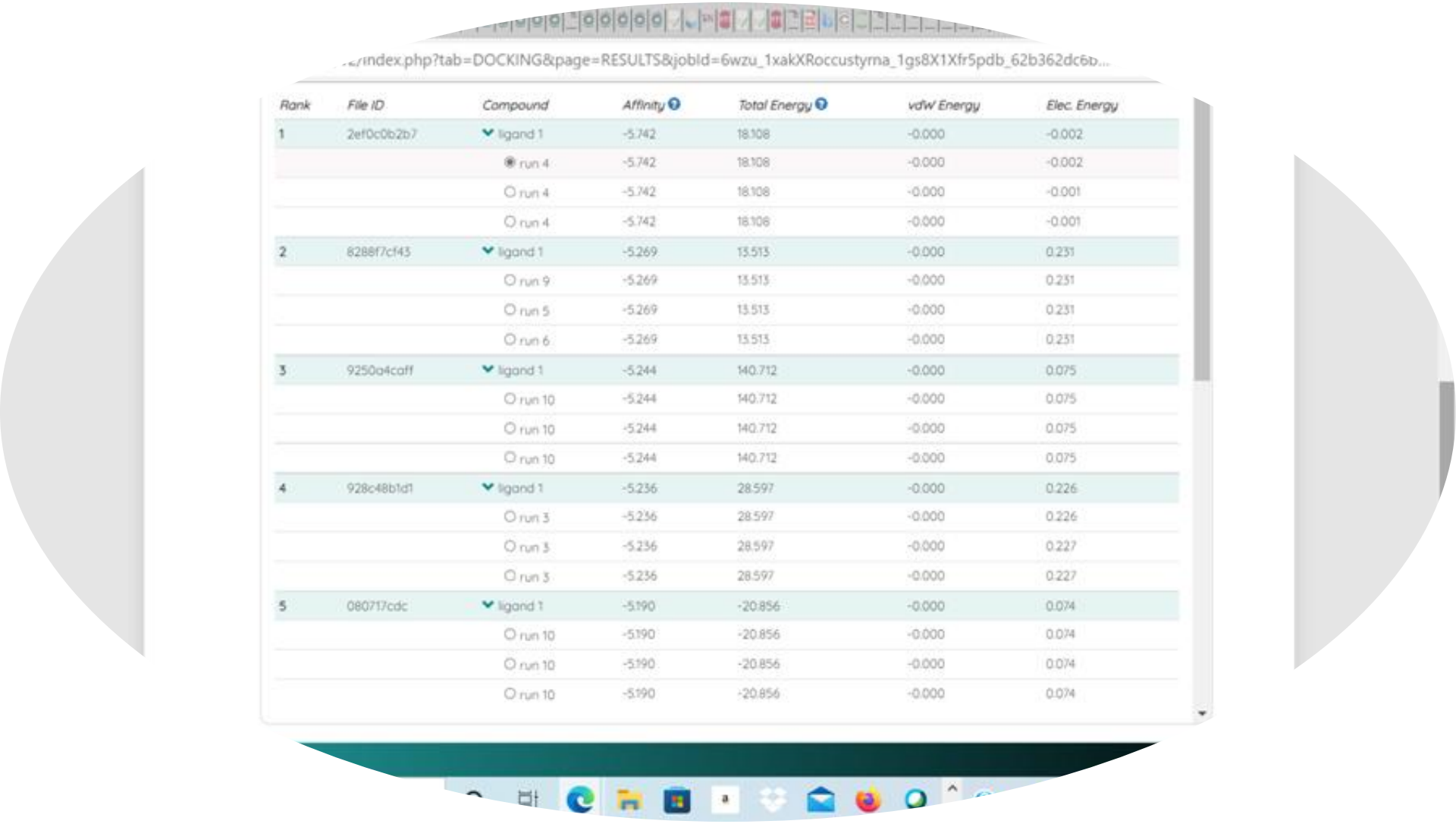
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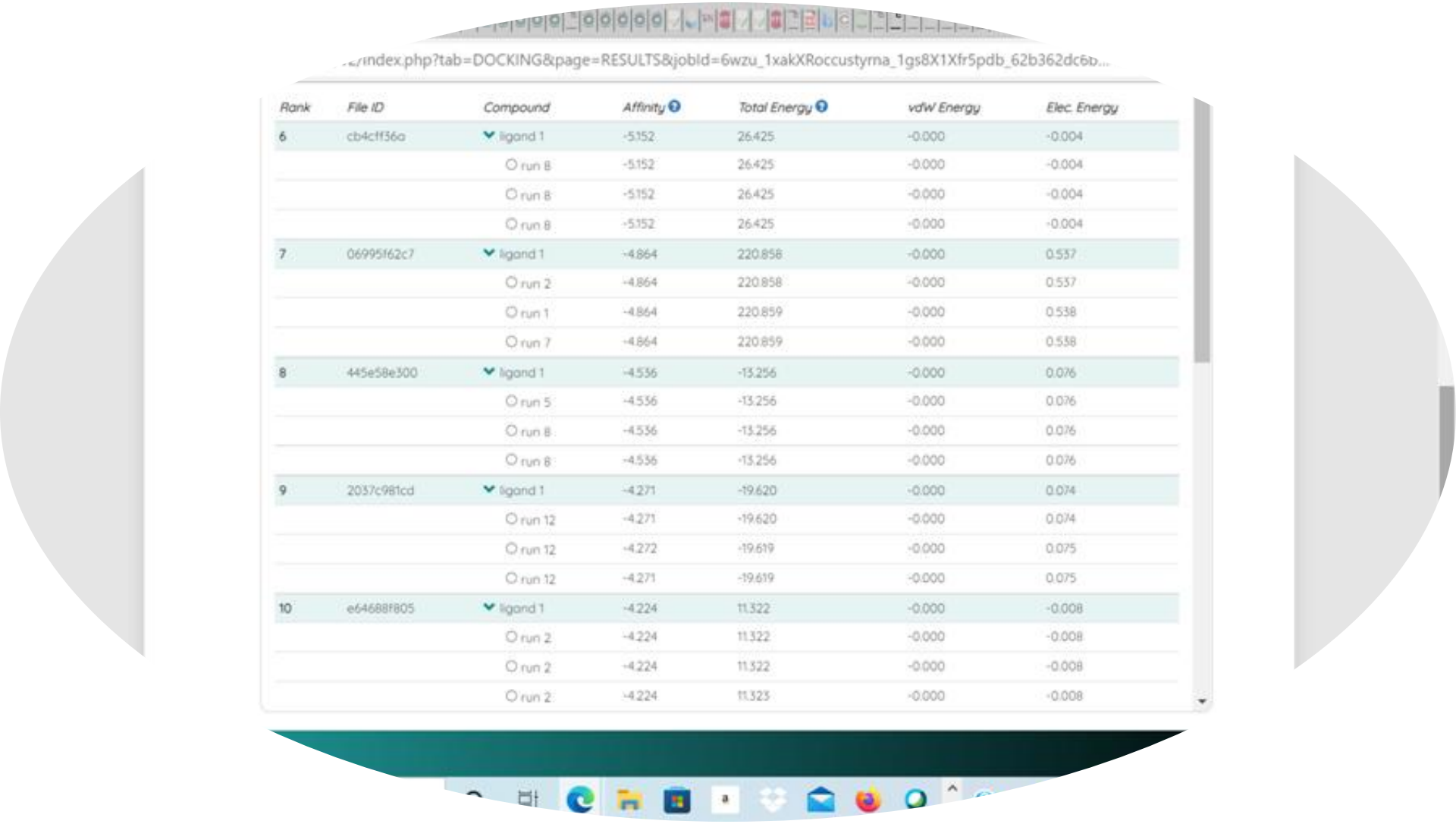
Rank File ID Compound Affinity Total Energy vdW Energy Elec. Energy
1 2ef0c0b2b7 ligand 1 -5.742 18.108 -0.000 -0.002
run 4 -5.742 18.108 -0.000 -0.002
run 4 -5.742 18.108 -0.000 -0.001
run 4 -5.742 18.108 -0.000 -0.001
2 8288f7cf43 ligand 1 -5.269 13.513 -0.000 0.231
run 9 -5.269 13.513 -0.000 0.231
run 5 -5.269 13.513 -0.000 0.231
run 6 -5.269 13.513 -0.000 0.231
3 9250a4caff ligand 1 -5.244 140.712 -0.000 0.075
run 10 -5.244 140.712 -0.000 0.075
run 10 -5.244 140.712 -0.000 0.075
run 10 -5.244 140.712 -0.000 0.075
4 928c48b1d1 ligand 1 -5.236 28.597 -0.000 0.226
run 3 -5.236 28.597 -0.000 0.226
run 3 -5.236 28.597 -0.000 0.227
run 3 -5.236 28.597 -0.000 0.227
5 080717cdc ligand 1 -5.190 -20.856 -0.000 0.074
run 10 -5.190 -20.856 -0.000 0.074
run 10 -5.190 -20.856 -0.000 0.074
run 10 -5.190 -20.856 -0.000 0.074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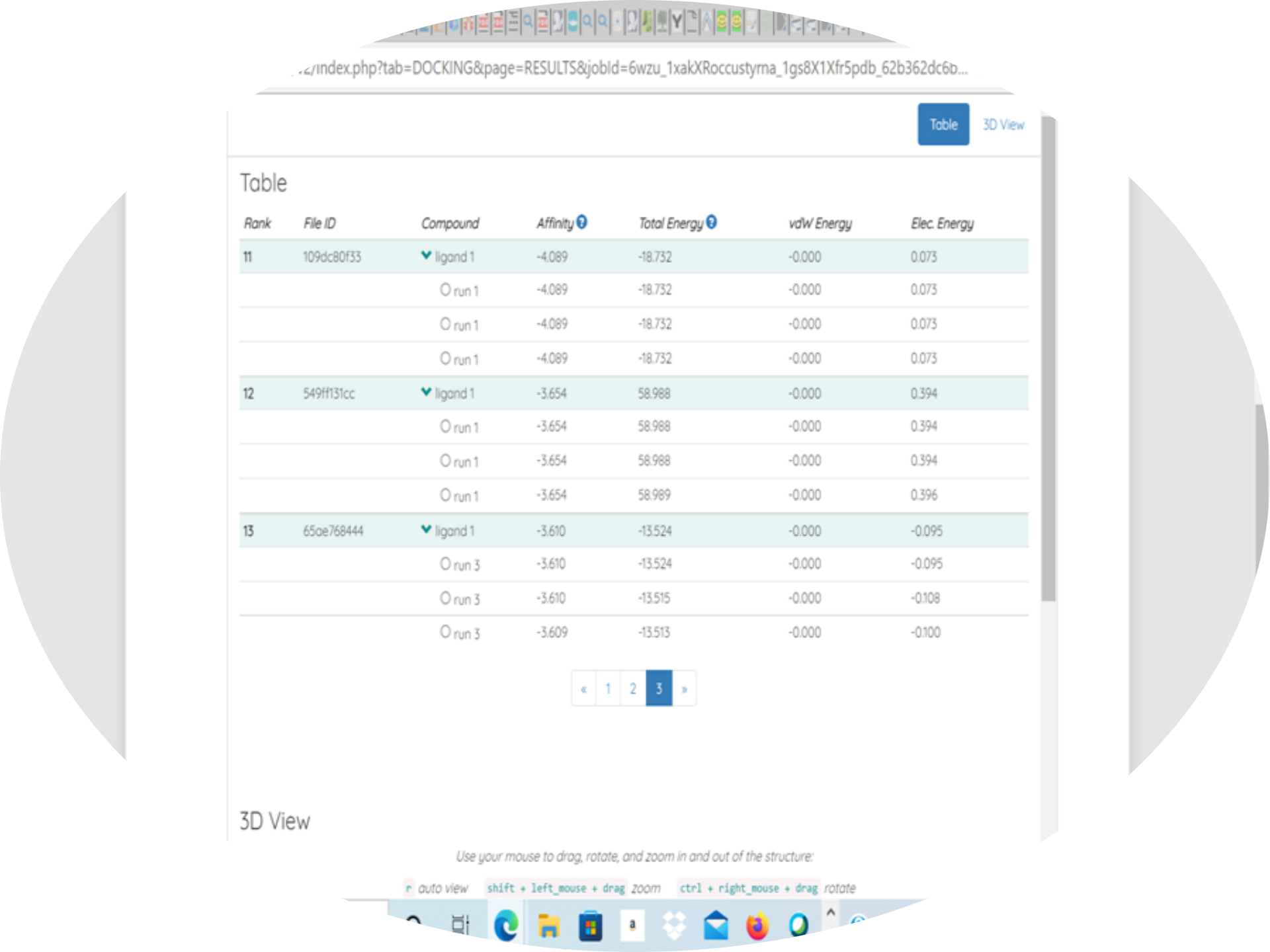
Rank File ID Compound Affinity Total Energy vdW Energy Elec. Energy
6 cb4cff36a ligand 1 -5.152 26.425 -0.000 -0.004
run 8 -5.152 26.425 -0.000 -0.004
run 8 -5.152 26.425 -0.000 -0.004
run 8 -5.152 26.425 -0.000 -0.004
7 06995f62c7 ligand 1 -4.864 220.858 -0.000 0.537
run 2 -4.864 220.858 -0.000 0.537
run 1 -4.864 220.859 -0.000 0.538
run 7 -4.864 220.859 -0.000 0.538
8 445e58e300 ligand 1 -4.536 -13.256 -0.000 0.076
run 5 -4.536 -13.256 -0.000 0.076
run 8 -4.536 -13.256 -0.000 0.076
run 8 -4.536 -13.256 -0.000 0.076
9 2037c981cd ligand 1 -4.271 -19.620 -0.000 0.074
run 12 -4.271 -19.620 -0.000 0.074
run 12 -4.272 -19.619 -0.000 0.075
run 12 -4.271 -19.619 -0.000 0.075
10 e64688f805 ligand 1 -4.224 11.322 -0.000 -0.008
run 2 -4.224 11.322 -0.000 -0.008
run 2 -4.224 11.322 -0.000 -0.008
run 2 -4.224 11.323 -0.000 -0.008



.../index.php?tab=DOCKING&page=RESULTS&jobId=6wzu_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b362dc6b...

Table 3D View

Table

Rank	File ID	Compound	Affinity	Total Energy	vdW Energy	Elec. Energy
11	109dc80f33	ligand 1	-4.089	-18.732	-0.000	0.073
		run 1	-4.089	-18.732	-0.000	0.073
		run 1	-4.089	-18.732	-0.000	0.073
		run 1	-4.089	-18.732	-0.000	0.073
12	549ff131cc	ligand 1	-3.654	58.988	-0.000	0.394
		run 1	-3.654	58.988	-0.000	0.394
		run 1	-3.654	58.988	-0.000	0.394
		run 1	-3.654	58.989	-0.000	0.396
13	65ae768444	ligand 1	-3.610	-13.524	-0.000	-0.095
		run 3	-3.610	-13.524	-0.000	-0.095
		run 3	-3.610	-13.515	-0.000	-0.108
		run 3	-3.609	-13.513	-0.000	-0.100

« 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=6wzu_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b362dc6b...
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]217:A.N - [LYS]217:A.CA (protein_310adc787_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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index.php?tab=DOCKING&page=RESULTS&jobId=6wzu_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b362dc6b...
bond: [LEU]185:A:CB - [LEU]185:A:CG (protein_310adc787_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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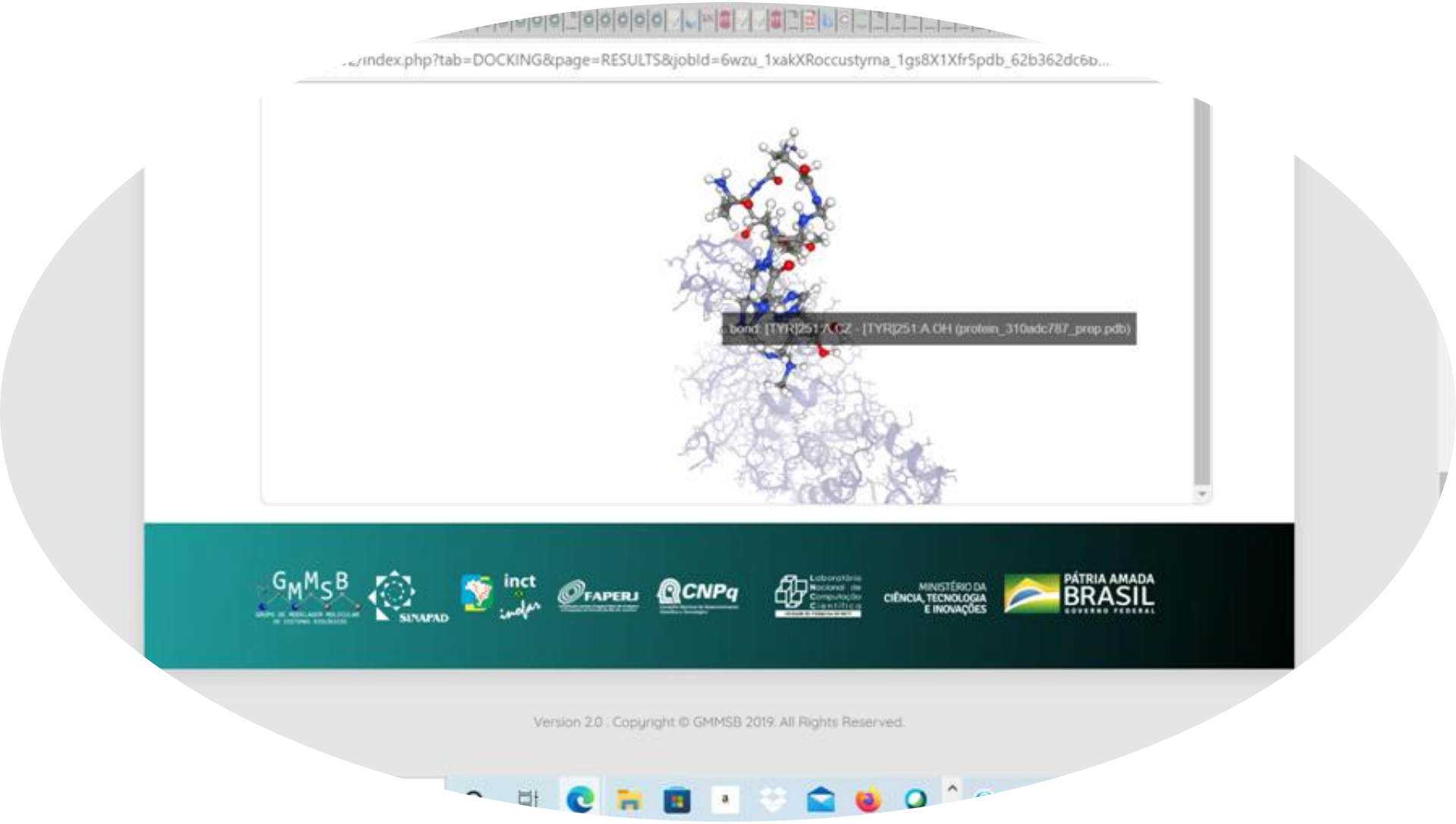
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bond: [TYR]251:A:CZ - [TYR]251:A:OH (protein_310adc787_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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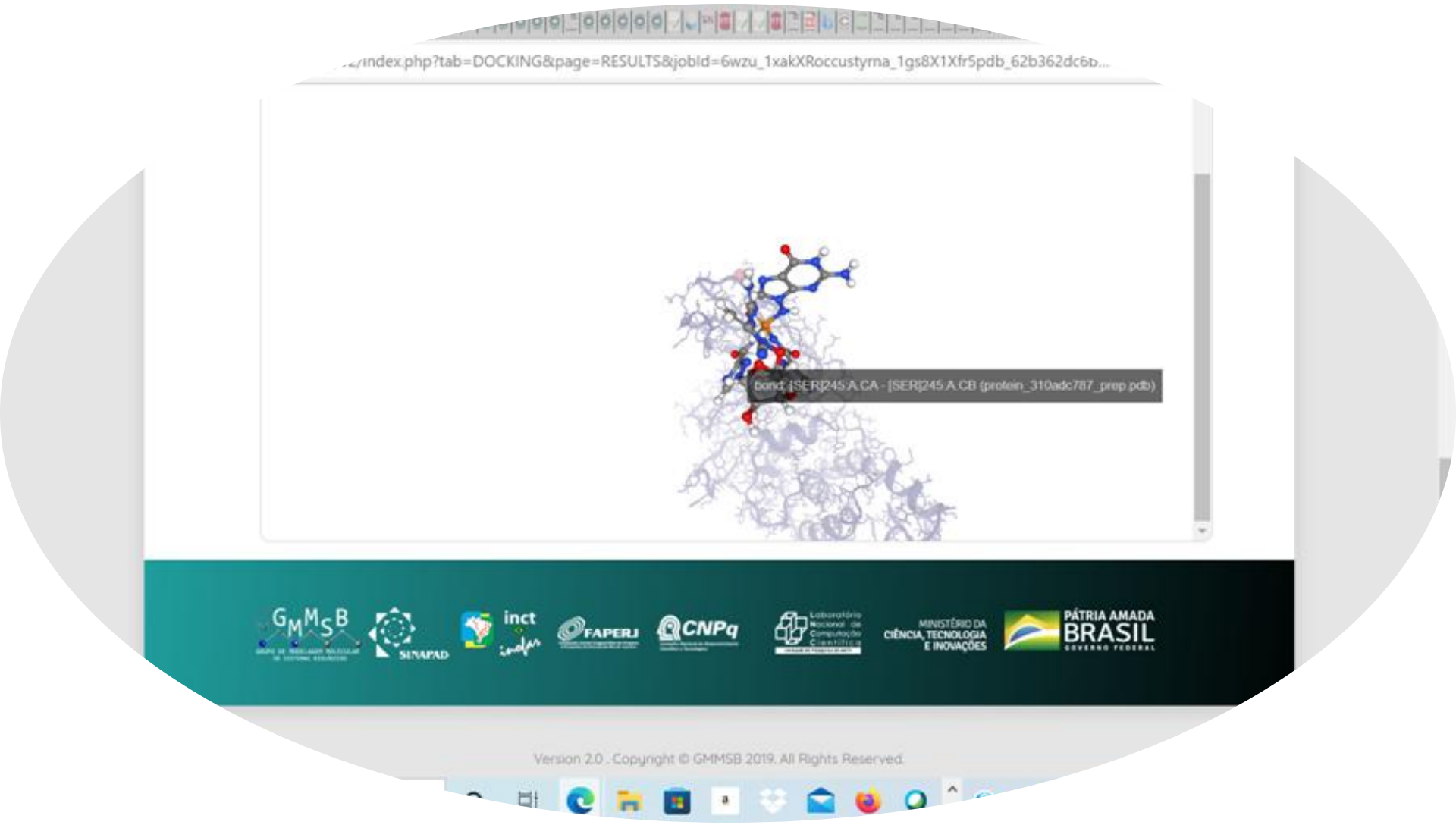
index.php?tab=DOCKING&page=RESULTS&jobId=6wzu_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b362dc6b...
bond: [SER]245.A.CA - [SER]245.A.CB (protein_310adc787_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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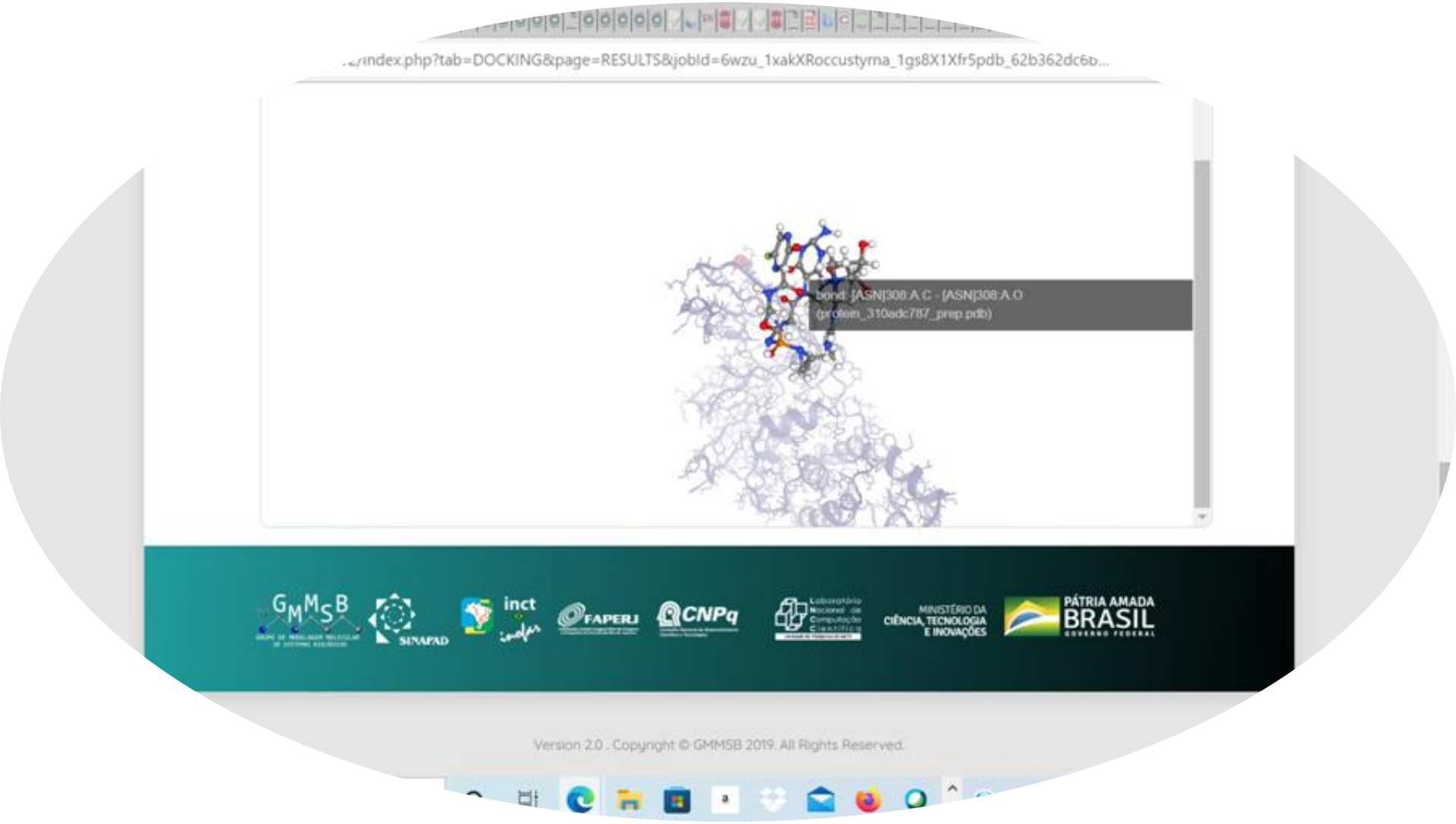
index.php?tab=DOCKING&page=RESULTS&jobId=6wzu_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b362dc6b...
bond: [ASN]308:A.C - [ASN]308:A.O
(protein_310adc787_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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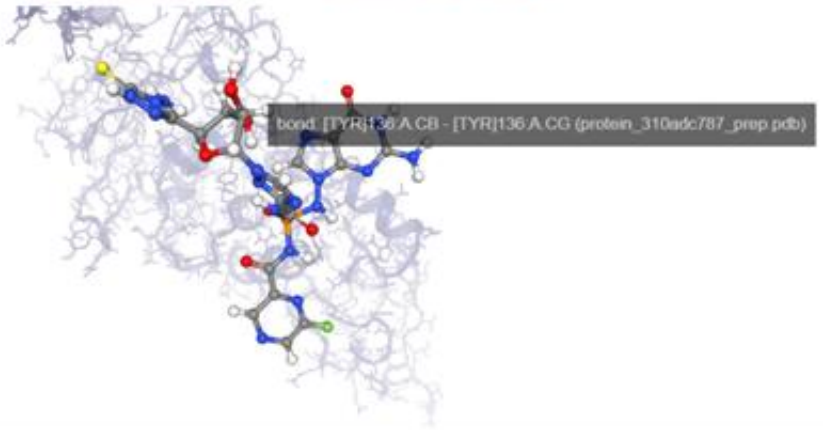
index.php?tab=DOCKING&page=RESULTS&jobId=6wzu_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b362dc6b...

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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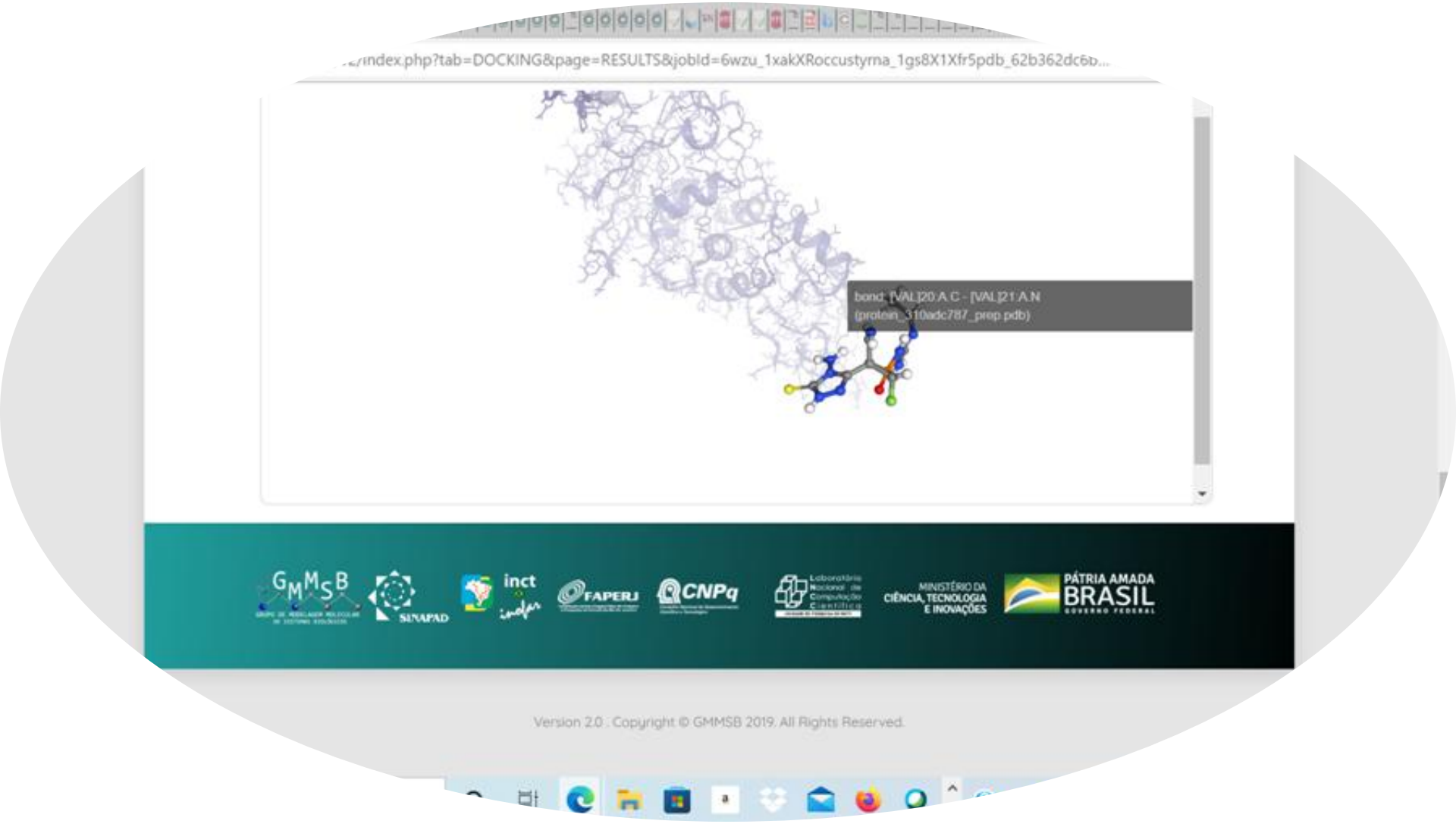
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bond: [VAL]20:A:C - [VAL]21:A:N
(protein_310adc787_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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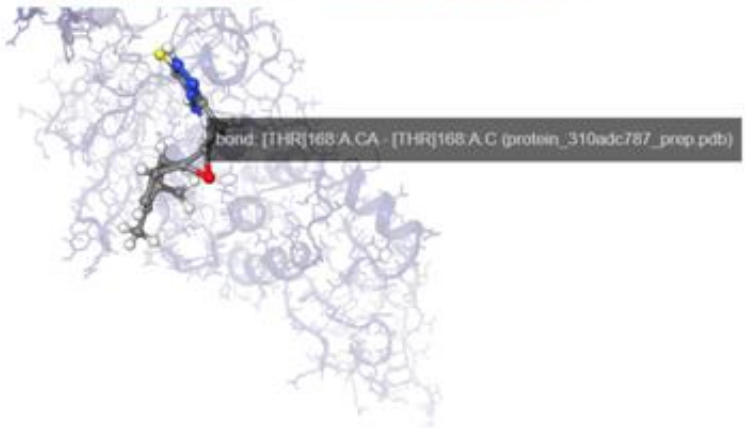
index.php?tab=DOCKING&page=RESULTS&jobId=6wzu_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b362dc6b...

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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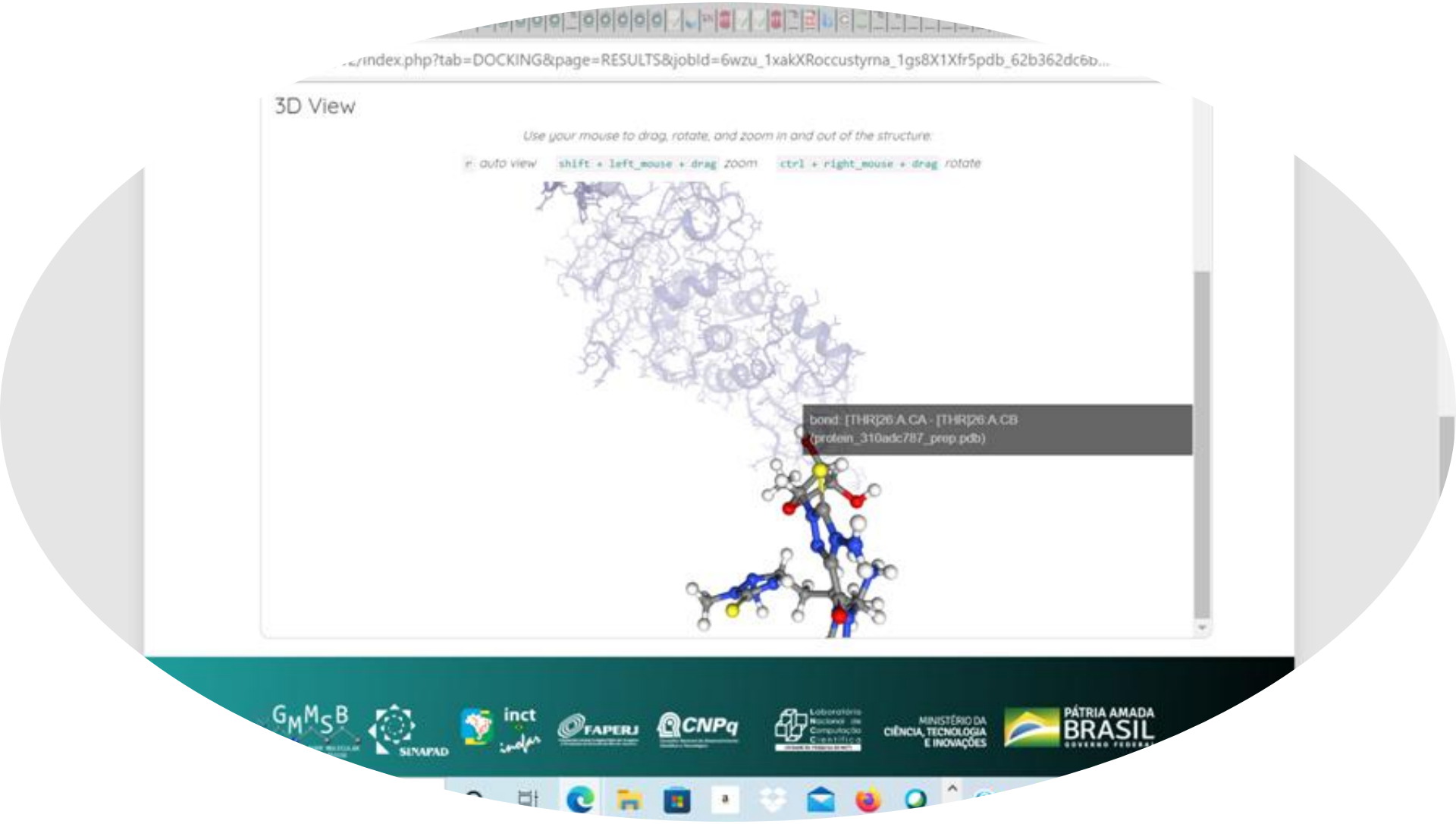
index.php?tab=DOCKING&page=RESULTS&jobId=6wzu_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b362dc6b...
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r: auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [THR]26:A:CA - [THR]26:A:CB
(protein_310adc787_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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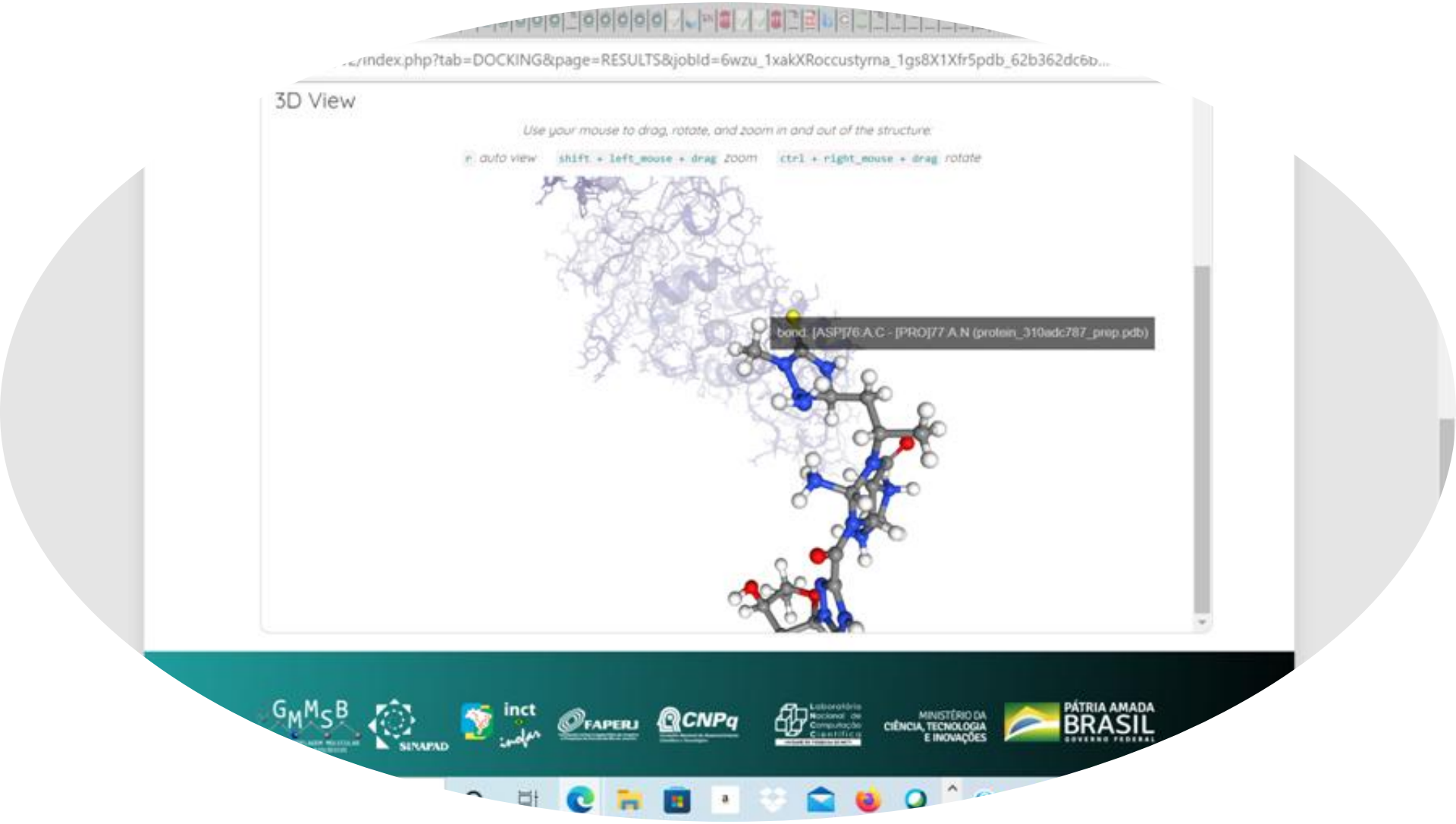
index.php?tab=DOCKING&page=RESULTS&jobId=6wzu_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b362dc6b...
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [ASP]76:A.C - [PRO]77:A.N (protein_310adc787_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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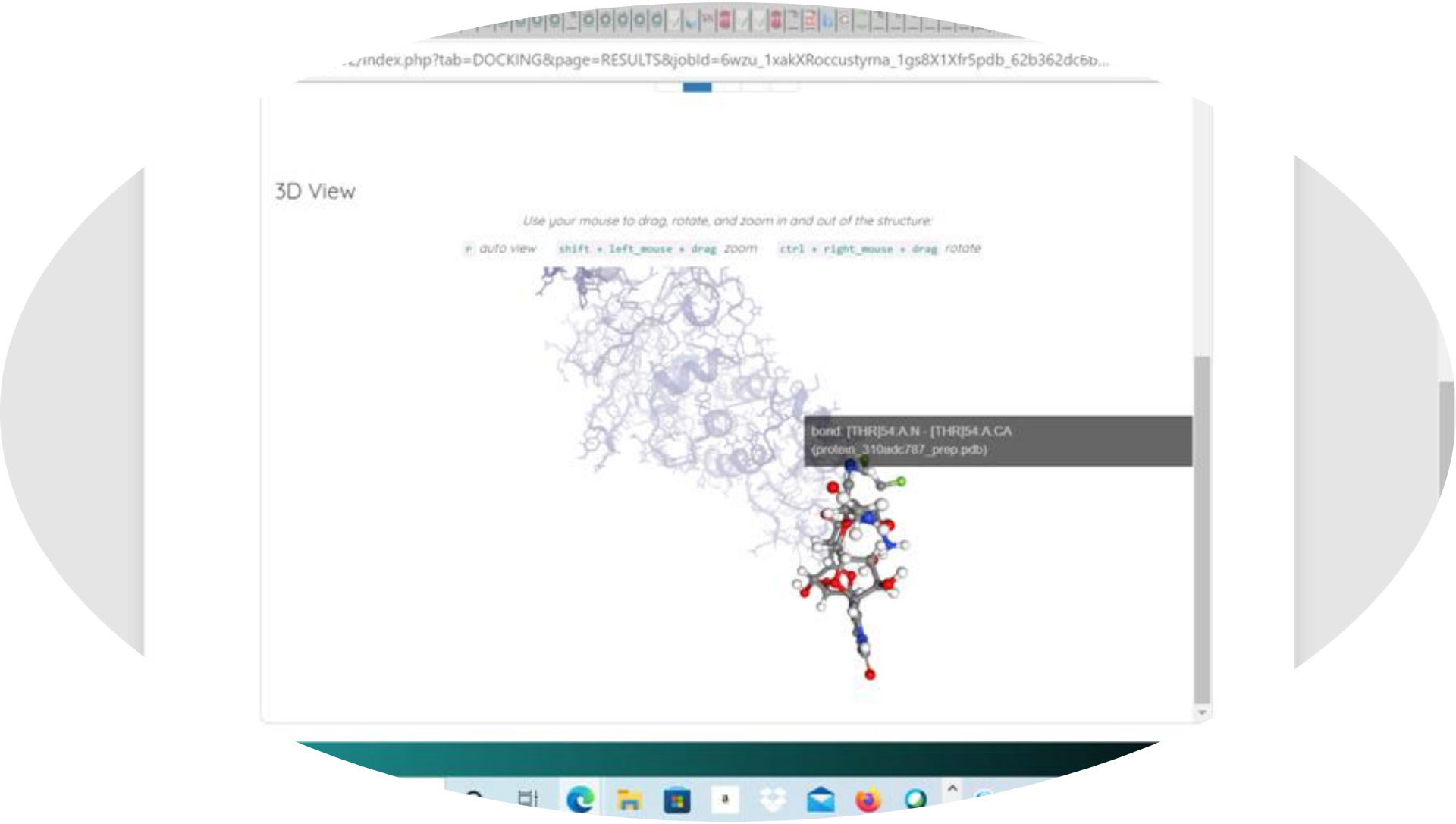
index.php?tab=DOCKING&page=RESULTS&jobId=6wzu_1xakXRoccustyrna_1gs8X1Xfr5pdb_62b362dc6b...
3D View
Use your mouse to drag, rotate, and zoom in and out of the structure.
r auto view
shift + left_mouse + drag zoom
ctrl + right_mouse + drag rotate
bond: [THR]54:A:N - [THR]54:A:CA
(protein_310adc787_prep.pdb)