index.php?tab=DOCKING&page=RESULTS&jobId=7tx5_RoccustyrnaTM_gs_convs_1XX2XXpdb_62b311a...

| Rank | File ID | Compound | Affinity | Total Energy | vdW Energy | Elec. Energy |
|---|---|---|---|---|---|---|
| 1 | b0e7429ea7 | ligand 1 | -6.750 | -56.300 | -10.928 | -21.840 |
| | | run 2 | -6.750 | -56.300 | -10.928 | -21.840 |
| | | run 4 | -7.566 | -54.877 | -9.330 | -24.185 |
| | | run 10 | -7.674 | -54.678 | -9.457 | -28.812 |
| 2 | a7a52ba6 | ligand 1 | -6.351 | -128.251 | -6.533 | -26.108 |
| | | run 12 | -6.351 | -128.251 | -6.533 | -26.108 |
| | | run 2 | -7.056 | -128.010 | -18.120 | -12.755 |
| | | run 12 | -6.323 | -126.579 | -0.881 | -29.779 |

« 1 »

## 3D View

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

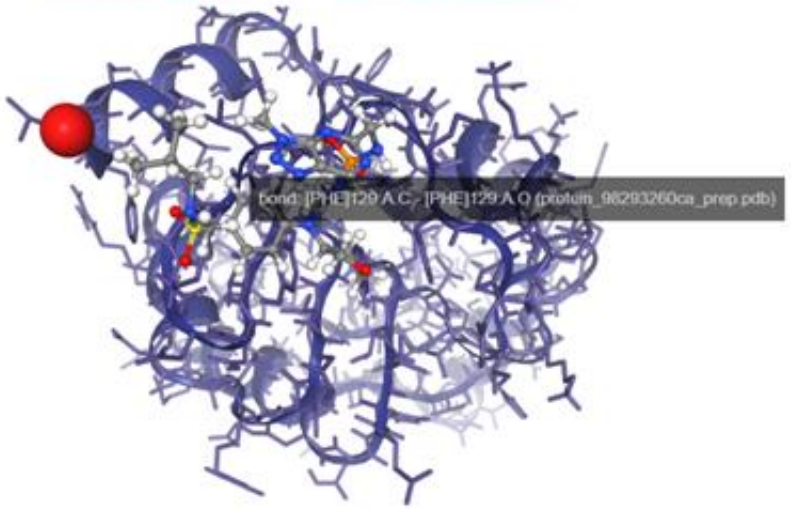
`r` *auto view* `shift + left_mouse + drag` *zoom* `ctrl + right_mouse + drag` *rotate*

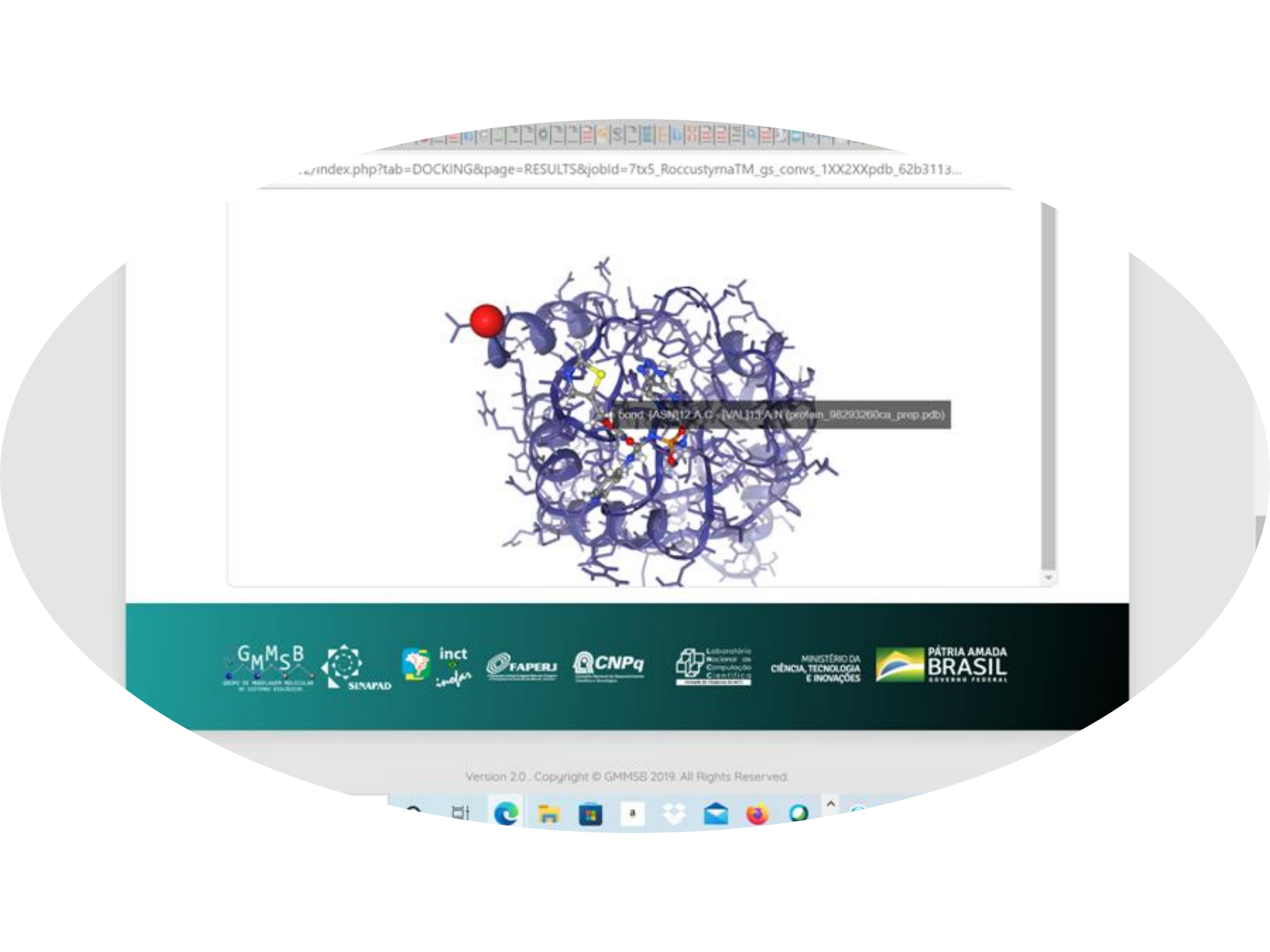
index.php?tab=DOCKING&page=RESULTS&jobId=7tx5_RoccustyrnaTM_gs_convs_1XX2XXpdb_62b3113...

## 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_RoccustyrnaTM_gs_convs_1XX2XXpdb_62b3113...
bond [ASN]12:A:C - [VAL]13:A:N (protein_98293260cs_prep.pdb)
GMMSB
SINAPAD
inct
FAPERJ
CNPq
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PÁTRIA AMADA BRASIL
GOVERNO FEDERAL
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