

## Specific information about the dynamics of the PDBs which have already been run and uploaded to MDposit.

This file contains information about specific errors encountered and solved when running / imaging and fitting the PDBs files (downloaded from MemProtMD).

PDBs	Information about the configuration of the Imaging	Status analysis (have passed the basic analyses: stable bonds, coherent bonds, RMSD?)	Uploaded	Website
	<p>It should be noted that when imaging these trajectories, the workflow parameters from the test RMSD from the MoDEL_CNS workflow by Daniel Beltrán was edited. *</p> <p>Moreover, depending of the trajectory we set a std of the RMSD between a value of 6 and 8.</p>			
<b>2k58</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-dev.mddbr.eu/#/id/64414f46d8203151cefd371f/overview">https://mdposit-dev.mddbr.eu/#/id/64414f46d8203151cefd371f/overview</a>
<b>2ksr</b>	<i>old protocol std=8</i>	<b>Correct</b>	Yes	<a href="https://mdposit-dev.mddbr.eu/#/id/644650e4df1b306958ae526d/overview">https://mdposit-dev.mddbr.eu/#/id/644650e4df1b306958ae526d/overview</a>
<b>2r4s</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-dev.mddbr.eu/#/id/644650e4df1b306958ae526d/overview">https://mdposit-dev.mddbr.eu/#/id/644650e4df1b306958ae526d/overview</a>

				<a href="#">/644651c375cb356a864857fe/overview</a>
<b>2ydo</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /6447dbd90fba421040cbf1ef/overview">https://mdposit-d ev.mddbr.eu/#/id /6447dbd90fba421040cbf1ef/overview</a>
<b>3eml</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /6447dc8b388f6326e0d21435/overview">https://mdposit-d ev.mddbr.eu/#/id /6447dc8b388f6326e0d21435/overview</a>
<b>3kj6</b>	<i>std=5, std=6</i>	<p><b>Incorrect (std=5)</b></p> <pre>Back off! I just backed up md.imaged. Reading frame 1 time 10.000 Dumping frame at t= 0 ps -&gt; frame 0 time 0.000 Last written: frame 0 time 0.0</pre> <p>----- Correcting topology -----  Finding safe bonds  Frame 10 / 10  WARNING: Default structure has wrong t  Searching safe bonds canonical frame  Frame 232 / 10001  Got it -&gt; Frame 232  The topology file has been modificat  -----  Running "snapshots"  Checking trajectory integrity  Frame 10000  FAIL: Sudden RMSD jump between frames  FAIL: Sudden RMSD jump between frames  FAIL: Sudden RMSD jump between frames <p>In VMD we don't see anything... well, just a little jump, but not significant.</p> <p><b>Incorrect (std=6)</b></p> <pre>Back off! I just backed up md.imaged. Reading frame 1 time 10.000 Dumping frame at t= 0 ps -&gt; frame 0 time 0.000 Last written: frame 0 time 0.0</pre> <p>----- Correcting topology -----  Finding safe bonds  Frame 10 / 10  WARNING: Default structure has wrong t  Searching safe bonds canonical frame  Frame 232 / 10001  Got it -&gt; Frame 232  The topology file has been modificat  -----  Running "snapshots"  Checking trajectory integrity  Frame 10000  FAIL: Sudden RMSD jump between frames <p>In VMD we don't see anything... well, just a little jump, but not significant.</p> </p></p>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /6447ddb161110c4a215c91f9/overview">https://mdposit-d ev.mddbr.eu/#/id /6447ddb161110c4a215c91f9/overview</a>

		<p><b>Correct</b></p> <p>As we see that it is well visually, we are going to make a trust. We have seen that for it to catch it correct all the frames we should put a std=6.2 but as it is practically insignificant we make a trust to this study and already.</p> <p><i>mwf -top md.tpr -traj md.xtc -char md.tpr -pr 4 -filt -i topology --trust cohonds intrajrity</i></p>		
3nya	std=5	<p><b>Correct</b></p>	Yes	<a href="https://mdposit-d.ev.mddbr.eu/#/id/644a3a280b169a4e220d884f/overview">https://mdposit-d.ev.mddbr.eu/#/id/644a3a280b169a4e220d884f/overview</a>
3p0g	std=5	<p><b>Correct</b></p>	Yes	<a href="https://mdposit-d.ev.mddbr.eu/#/id/644a3af158458a67899273c9/overview">https://mdposit-d.ev.mddbr.eu/#/id/644a3af158458a67899273c9/overview</a>
3pbl	std=5	<p><b>Correct</b></p>	Yes	<a href="https://mdposit-d.ev.mddbr.eu/#/id/644a3b671c08a47680458b4c/overview">https://mdposit-d.ev.mddbr.eu/#/id/644a3b671c08a47680458b4c/overview</a>
3pds	std=5, std=6	<p><b>Incorrect</b></p> <pre> Precision of md.inaged.rot.xtc is 0.001 (nm) Back Off! I just backed up md.inaged.rot.dr Reading frame 1 time 10.000 Dumpling frame at t= 0 ps -&gt; frame 0 time 0.000 Last written: frame 0 time 0.000  ----- Correcting topology ----- Finding safe bonds Frame 10 / 10 WARNING: Default structure has wrong bonds Searching safe bonds canonical frame Frame 2 / 10001 Got it -&gt; Frame 2 The topology file has been modified -&gt; ----- Running "snapshots" Checking trajectory integrity Frame 10000 FAIL: Sudden RMSD jump between frames 6671 Failed RMSD checking (mwf) lnartinv@orozco701:~/Escritorio/ventan </pre>	Yes	<a href="https://mdposit-d.ev.mddbr.eu/#/id/644a3be445f0eb06436c8b72/overview">https://mdposit-d.ev.mddbr.eu/#/id/644a3be445f0eb06436c8b72/overview</a>

		<p>When we visualize it in vmd everything seems to be correct.</p> <p>...</p> <p><b>Correct (std=6)</b></p>		
<b>3qak</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a3c5db26b5 c135c1edee1/ov erview">https://mdposit-d ev.mddbr.eu/#/id /644a3c5db26b5 c135c1edee1/ov erview</a>
<b>3rze</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a3cc87f188 71ed442c565/ov erview">https://mdposit-d ev.mddbr.eu/#/id /644a3cc87f188 71ed442c565/ov erview</a>
<b>3vg9</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a3d2bd2b43 f298d1d3940/ov erview">https://mdposit-d ev.mddbr.eu/#/id /644a3d2bd2b43 f298d1d3940/ov erview</a>
<b>3vga</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a3d97ca09c 034829ccd33/ov erview">https://mdposit-d ev.mddbr.eu/#/id /644a3d97ca09c 034829ccd33/ov erview</a>
<b>4cof</b>	<i>std=6</i>	<p><b>ERROR BLAST</b></p> <pre> ===== Loading "topoblast" Checking trajectory integrity Frame 10000 Executing specific dependencies: ['topology'] Loading charges Charges in the "topology.trp" file will be used Loading map References for PDB code 4cof: P20472 Using also references related to PDB ids from inputs.json Aligning chain A with P20472 reference sequence Not valid alignment Reference summary: A -&gt; 2 Throwing blast... Result: P20472 Using also references from blast Reference summary: A -&gt; 20 BLAST failed to find a matching reference sequence for at least one (mnr) (mnr) (mnr) (mnr) (mnr) (mnr) (mnr) (mnr) (mnr) (mnr) </pre> <p><b>Corrected</b></p>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /6458fc9a39473 d49cf4972e9/ov erview">https://mdposit-d ev.mddbr.eu/#/id /6458fc9a39473 d49cf4972e9/ov erview</a>
<b>4eiy</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a3e2d6bf8af 4347a808cf/over view">https://mdposit-d ev.mddbr.eu/#/id /644a3e2d6bf8af 4347a808cf/over view</a>

<b>4gbr</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a63ec05c7f 3693df9d870/ov erview">https://mdposit-d ev.mddbr.eu/#/id /644a63ec05c7f 3693df9d870/ov erview</a>
<b>4mq5</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a64621c907 e7b16025d4f/ov erview">https://mdposit-d ev.mddbr.eu/#/id /644a64621c907 e7b16025d4f/ov erview</a>
<b>4mqt</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a662d9ebb3 531bccaed24/ov erview">https://mdposit-d ev.mddbr.eu/#/id /644a662d9ebb3 531bccaed24/ov erview</a>
<b>4ug2</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a66935604b f3da7eee0f5/ove rview">https://mdposit-d ev.mddbr.eu/#/id /644a66935604b f3da7eee0f5/ove rview</a>
<b>4uhr</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a66fde3a94 049332ab54b/ov erview">https://mdposit-d ev.mddbr.eu/#/id /644a66fde3a94 049332ab54b/ov erview</a>
<b>5cxv</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a6762b56e9 853f4271cc2/ov erview">https://mdposit-d ev.mddbr.eu/#/id /644a6762b56e9 853f4271cc2/ov erview</a>
<b>5d5b</b>	<i>std=6</i>	<p><b>Incorrect</b></p> <pre>Running "snapshots" Checking trajectory integrity Frame 2209 Frame 10000 FAIL: Sudden RMSD jump between Failed RMSD checking</pre> <p>Visually with vmd I don't see anything serious. I see that there is a mini jump between the 806 and 807 but well, I consider that it is small and that it is nothing relevant.</p>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a67dee7db1 660e391f913/ov erview">https://mdposit-d ev.mddbr.eu/#/id /644a67dee7db1 660e391f913/ov erview</a>

		<p><b>Correct</b></p> <p>Since I consider it to be insignificant, I make it a trust</p> <p><i>mwf -top md.tpr -traj md.xtc -char md.tpr -pr 4 -filt -i topology --trust cohbonds intrajrity</i></p>		
<b>5iu8</b>	<i>old protocol std=8</i>	<b>Correct</b> (con mensaje de topo arreglado)	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a68726757e 26f7d16c337/overview">https://mdposit-d ev.mddbr.eu/#/id /644a68726757e 26f7d16c337/overview</a>
<b>5iua (</b>	<i>old protocol std=8</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a69accd848 50f07f31483/overview">https://mdposit-d ev.mddbr.eu/#/id /644a69accd848 50f07f31483/overview</a>
<b>5jqh</b>	<i>std=6</i>	<b>Correct</b>	No, interprone error	
<b>5jtb</b>	<i>old protocol std=8</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a6a9a568b0 12676b22d7c/overview">https://mdposit-d ev.mddbr.eu/#/id /644a6a9a568b0 12676b22d7c/overview</a>
<b>5mzp</b>	<i>std=8 old protocol</i>	Correct	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a6b18a0587 f330bd54c66/overview">https://mdposit-d ev.mddbr.eu/#/id /644a6b18a0587 f330bd54c66/overview</a>
<b>5n2r</b>	<i>std=5</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /644a6bbe7f5f 42cb915159/overview">https://mdposit-d ev.mddbr.eu/#/id /644a6bbe7f5f 42cb915159/overview</a>



<b>5wf5</b>	<i>old protocol std=8</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /6458be035d8cd 640f57f489d/ove rview">https://mdposit-d ev.mddbr.eu/#/id /6458be035d8cd 640f57f489d/ove rview</a>
<b>5wf6</b>	<i>old protocol std=8</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /6458be7a0b416 a421f0ee152/ov erview">https://mdposit-d ev.mddbr.eu/#/id /6458be7a0b416 a421f0ee152/ov erview</a>
5wiu	<i>std=5, std=6</i>	<p><b>Incorrect (std=5)</b> It tells me there is an RMSD error between 186 and 187 but when I look at it in vmd I don't see anything.</p> <p>...</p> <p><b>Incorrect (std=6)</b> Same RMSD error between 186 and 187.</p> <p>...</p> <p><b>Correct</b> As we can see that it looks good visually, we are going to make it a trust</p> <p><i>mwf -top md.tpr -traj md.xtc -char md.tpr -pr 4 -filt -i topology --trust cohbonds intrajrity</i></p>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /6458bede362e6 a4327ca1c54/ov erview">https://mdposit-d ev.mddbr.eu/#/id /6458bede362e6 a4327ca1c54/ov erview</a>
<b>5wiv</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /6458bf913fd7b5 443386745b/ove rview">https://mdposit-d ev.mddbr.eu/#/id /6458bf913fd7b5 443386745b/ove rview</a>
<b>5x7d</b>	<i>I do not remember</i>	<b>Incorrect:</b> <b>ValueError:</b> <b>Something went</b>	Yes	<a href="https://mdposit-d ev.mddbr.eu/#/id /6458bffaab2b6c">https://mdposit-d ev.mddbr.eu/#/id /6458bffaab2b6c</a>



		wrong with the Uniprot request (error 500) ... <b>Correct</b>		<a href="https://mdposit-d-ev.mddbr.eu/#/id/4540781084/overview">4540781084/overview</a>
<b>Vuelvo a tirar el analyzer y workflow para estas a ver si lo de 100 ns se va así:</b>				
<b>5yc8</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d-ev.mddbr.eu/#/id/6458e25c8b6c0646fca4807e/overview">https://mdposit-d-ev.mddbr.eu/#/id/6458e25c8b6c0646fca4807e/overview</a>
<b>5zk3</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d-ev.mddbr.eu/#/id/645901330e87044ae5c09842/overview">https://mdposit-d-ev.mddbr.eu/#/id/645901330e87044ae5c09842/overview</a>
<b>5zk8</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d-ev.mddbr.eu/#/id/645cb041ba067e16ecec3e59/overview">https://mdposit-d-ev.mddbr.eu/#/id/645cb041ba067e16ecec3e59/overview</a>
<b>5zkb</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d-ev.mddbr.eu/#/id/645cb0aba835ae180666c357/overview">https://mdposit-d-ev.mddbr.eu/#/id/645cb0aba835ae180666c357/overview</a>
<b>6a93</b>	<i>new protocol std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d-ev.mddbr.eu/#/id/645cb0e47d1e96191cbd6def/overview">https://mdposit-d-ev.mddbr.eu/#/id/645cb0e47d1e96191cbd6def/overview</a>
<b>6a94</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d-ev.mddbr.eu/#/id/645cb11591eec41a33e043dc/overview">https://mdposit-d-ev.mddbr.eu/#/id/645cb11591eec41a33e043dc/overview</a>
<b>6aqf</b>	<i>new protocol</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d-ev.mddbr.eu/#/id/645cb11591eec41a33e043dc/overview">https://mdposit-d-ev.mddbr.eu/#/id/645cb11591eec41a33e043dc/overview</a>

	<i>std=8</i>			<a href="https://ev.mddbr.eu/#/id/645cb1559bc81a1b4e777253/overview">ev.mddbr.eu/#/id/645cb1559bc81a1b4e777253/overview</a>
<b>6bqg</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d.ev.mddbr.eu/#/id/645cb172297c021c5a68a227/overview">https://mdposit-d.ev.mddbr.eu/#/id/645cb172297c021c5a68a227/overview</a>
<b>6bqh</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d.ev.mddbr.eu/#/id/645cb197563b941d6bce49ee/overview">https://mdposit-d.ev.mddbr.eu/#/id/645cb197563b941d6bce49ee/overview</a>
<b>6cm4</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d.ev.mddbr.eu/#/id/645cb1b81917f61e7869e58c/overview">https://mdposit-d.ev.mddbr.eu/#/id/645cb1b81917f61e7869e58c/overview</a>
<b>4cof</b>	<i>std=6</i>	<b>Correct</b>	Yes	<a href="https://mdposit-d.ev.mddbr.eu/#/id/6458fc9a39473d49cf4972e9/overview">https://mdposit-d.ev.mddbr.eu/#/id/6458fc9a39473d49cf4972e9/overview</a>

\* The previous protocol before being edited in this project was the following:

Al final he cambiado el protocolo (*Old protocol*) de esto:

```
# Run Gromacs

p = Popen([
    "echo",
    center_selection_name,
    "System",
], stdout=PIPE)
logs = run([
    "gmx",
    "trjconv",
    "-s",
    input_tpr_filename,
    "-f",
    input_trajectory_filename,
    "-o",
    output_trajectory_filename,
    "-pbc",
    'res', # Note that the 'res' option requires a tpr to be passed
    '-center',
    '-ur',
    'compact',
    '-n',
    center_selection_filename,
    '-quiet'
], stdin=p.stdout, stdout=PIPE).stdout.decode()
p.stdout.close()
```

When doing the imaging of these proteins it was seen that a great large numbers of proteins were not correctly imaged. Therefore, it was changed from the above code to the following code:

```
# Run Gromacs

p = Popen([
    "echo",
    center_selection_name,
    "System",
], stdout=PIPE)
logs = run([
    "gmx",
```

```

        "trjconv",
        "-s",
        input_tpr_filename,
        "-f",
        input_trajectory_filename,
        '-o',
        output_trajectory_filename,
        '-center',
        '-pbc',
        'nojump',
        '-n',
        center_selection_filename,
        '-quiet'
    ], stdin=p.stdout, stdout=PIPE).stdout.decode()
p.stdout.close()

# Run Gromacs
p = Popen([
    "echo",
    "System",
], stdout=PIPE)
logs = run([
    "gmx",
    "trjconv",
    "-s",
    input_tpr_filename,
    "-f",
    output_trajectory_filename,
    '-o',
    output_trajectory_filename,
    '-pbc',
    'res', # Note that the 'res' option requires a tpr to be passed
    '-n',
    center_selection_filename,
    '-quiet'
], stdin=p.stdout, stdout=PIPE).stdout.decode()
p.stdout.close()

```