IQmol: Troubleshooting

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Known problems and glitches:

1. When configuring servers, follow the instructions **precisely**. If you get crashes when configuring the server, delete the configuration and start over again.

2. ‘Symmetrize’ function sometimes causes IQmol to crash.

3. If IQmol stops working (warnings like “cannot create a directory”) RESTART IQmol and try again.

4. If connection is poor, IQmol may show the running job as failed. In this case, or IQmol crashed, or your job is too long, you can copy the output and checkpoint files manually (by sftp) to your laptop and then open them by IQmol (may need to rename checkpoint files).

5. The job name is assigned when you select a working directory on the server. After the job finishes, IQmol will ask your permission to copy the files from the server. The name of the directory on your laptop should match the name of the directory on the server (i.e., the job name) **precisely**. If they do not match, you will get “no valid data found in …” error message. The files are actually OK and are copied to you laptop. You can open them individually with “Open…” command.
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