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| --- | --- | --- |
| **Sr. No** | **Complex Name** | **Simulation Status** |
| 1 | Aminostep2012 | Complete |
| 2 | Aminostep2016 | Complete |
| 3 | Aminotob2016 | Complete |
| 4 | Ndxgyra1996 | Complete |
| 5 | Ndxgyra2018 | Complete |
| 6 | Pbpmez2018 | Malformatted ligand. Acpype crashed |
| 7 | Pbppen1999 | Malformatted ligand. Acpype crashed |
| 8 | Pbppen2018 | Malformatted ligand. Acpype crashed |
| 9 | Levgyra2018 | Malformatted ligand. Acpype crashed |
| 10 | Levparc2018 | **Protein Too big** |
| 11 | Ndxparc1999 | **Protein Too big** |
| 12 | Ndxparc2018 | **Protein Too big** |

Diagnosis:

Problem with the PDBs of the following ligands: MEZ Need to download the structures from ncbi, instead of using rdkit to generate from SMILES.

Docking of Pbppen1999 corrupted the PEN ligand somehow. Probably should rerun after downloading these structures...

This seems to have happened to all the ligands :(

The docked ligands chosen for simulation need to be deprotonated and re-protonated properly using rdkit.