

RoseTTAFold

```
/fs00/software/rosettafold/1.1.0
```

Diagram illustrating a container environment setup. The container is represented by a large rectangle divided into two sections. The top section contains a terminal window with the command 'apptainer bind home RoseTTAFold folding conda'. The bottom section contains a terminal window with the command '--no-home'.

```
#BSUB -J RoseTTAFold
#BSUB -q gpu
#BSUB -n 8
#BSUB -gpu num=1

##### Configurie Numpy threads #####

export OMP_NUM_THREADS="$LSB_DJOB_NUMPROC"
export MKL_NUM_THREADS="$LSB_DJOB_NUMPROC"

##### Definition #####

ROSETTAFOLD_DATADIR=/bbfs/data/rosettafold      # path to RoseTTAFold data (host)
ROSETTAFOLD_IMAGE=RoseTTAFold-1.1.0.sif        # path to RoseTTAFold image (host)
ROSETTAFOLD_APPDIR=/app/RoseTTAFold            # path to RoseTTAFold working directory (container)

##### Database #####

UNIREF30_DB=$ROSETTAFOLD_DATADIR/UniRef30_2020_06
BFD_DB=$ROSETTAFOLD_DATADIR/bfd
PDB100_DB=$ROSETTAFOLD_DATADIR/pdb100_2021Mar03

##### Example #####

RUN_ROSETTAFOLD="apptainer run --bind $UNIREF30_DB:$ROSETTAFOLD_APPDIR/UniRef30_2020_06 \
--bind $BFD_DB:$ROSETTAFOLD_APPDIR/bfd \
--bind $PDB100_DB:$ROSETTAFOLD_APPDIR/pdb100_2021Mar03 \
--nv $ROSETTAFOLD_IMAGE"
```

For monomer structure prediction (e2e)

```
${RUN_ROSETTAFOLD} $ROSETTAFOLD_APPDIR/run_e2e_ver.sh $ROSETTAFOLD_APPDIR/example/input.fasta  
output/
```

For monomer structure prediction (pyrosetta)

```
${RUN_ROSETTAFOLD} $ROSETTAFOLD_APPDIR/run_pyrosetta_ver.sh $ROSETTAFOLD_APPDIR/example/input.fasta  
output/
```

For complex modeling

```
${RUN_ROSETTAFOLD} python $ROSETTAFOLD_APPDIR/network/predict_complex.py \  
-i $ROSETTAFOLD_APPDIR/example/complex_modeling/paired.a3m \  
-o output/ -Ls 218 310
```

For PPI screening using faster 2-track version (example input and output are at example/complex_2track)

```
${RUN_ROSETTAFOLD} python $ROSETTAFOLD_APPDIR/network_2track/predict_msa.py \  
-msa $ROSETTAFOLD_APPDIR/example/complex_2track/input.a3m \  
-npz output/complex.npz -L1 218
```

Revision #2

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