

RoseTTAFold

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

Diagram illustrating the environment setup for the RoseTTAFold application:

- The container environment (apptainer) is bound to the host's /home directory.
- The container environment contains the RoseTTAFold application.
- The container environment is linked to the host's conda environment.
- The container environment is configured with the --no-home flag.

```
#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=/fsb/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
```

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