Rosetta Input/Output

Cristina Elisa Martina
2025 Rosetta Workshop
Meiler Lab

How do I get Rosetta?

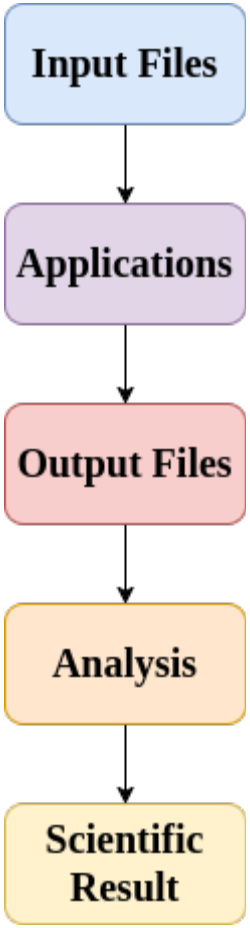
Download Rosetta:
https://rosettacommons.org/software/download/

Current release: Rosetta version 3.14

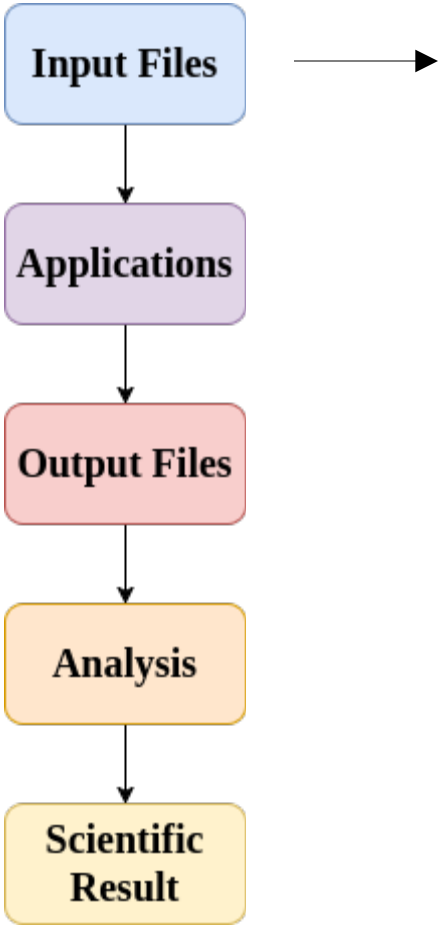
All tutorials here use version 3.14

Links to documentation, forum and demos:
https://docs.rosettacommons.org/docs/latest/Home
https://docs.rosettacommons.org/demos/latest/Home

General Workflow



Input Files

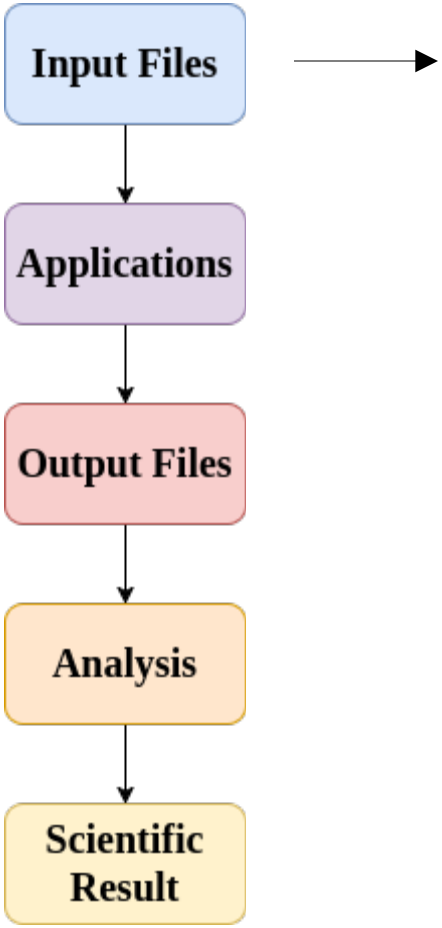


Molecules:
Protein structure (pdb, silent files)
Protein sequence (fasta file)
Ligand structures (pdb, sdf file)

Application-specific inputs:
Span file (define residues in membrane)
Loops file (identify loop residues)
Param file (NCAA or small molecules)
Res file (residues to design)

Options:
-nstruct 1000
-score:weights XXX.wts

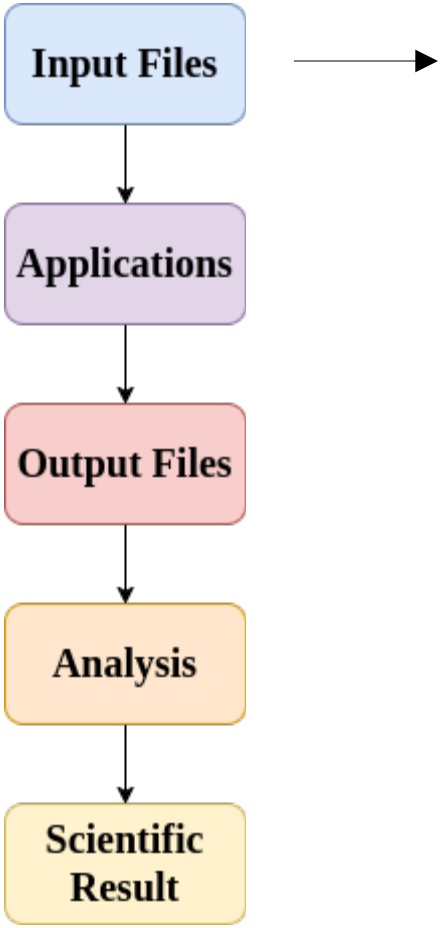
Input Files



Input options:
-parser:protocol XXX.xml
-in:file:s XXX.pdb
-in:file:fasta XXX.fasta
-in:file:silent XXX.silent
-in:file:extra_res_fa XXX.params

Output options:
-out:file:silent XXX.silent
-out:file:scorefile XXX.sc

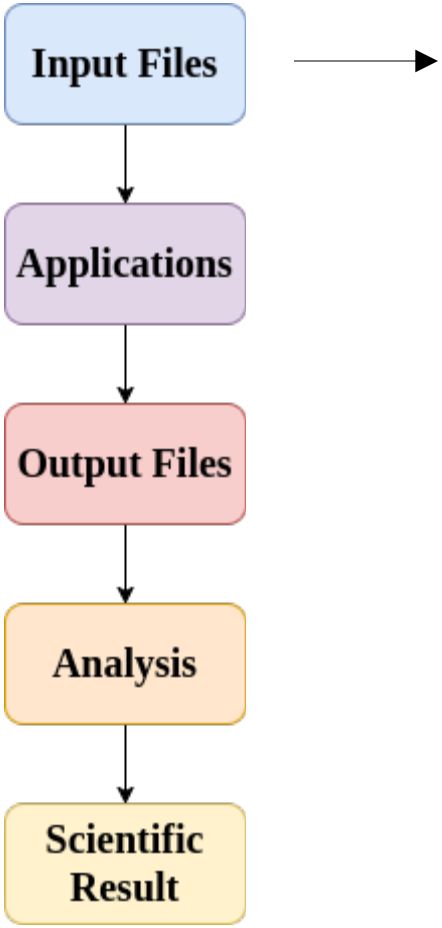
Input Files



Protocols can get complicated:

$ROSETTA/main/source/bin/AbinitioRelax.linuxgccrelease -database ../../rosetta_database -in:file:fasta ./input_files/1elwA.fasta -in:file:native ./input_files/1elw.pdb -in:file:frag3 ./input_files/aa1elwA03_05.200_v1_3 -in:file:frag9 ./input_files/aa1elwA09_05.200_v1_3 -abinitio:relax -relax:fast -abinitio::increase_cycles 10 -abinitio::rg_reweight 0.5 -abinitio::rsd_wt_helix 0.5 -abinitio::rsd_wt_loop 0.5 -use_filterstrue -psipred_ss2 ./input_files/1elwA.psipred_ss2 -kill_hairpins -out:file:silent 1elwA_silent.out -nstruct 10

Input Files

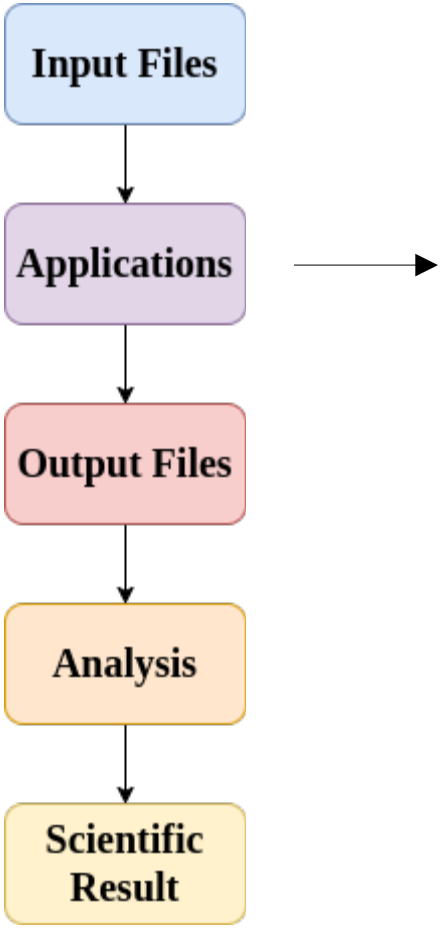


But you can use @options.txt:

$ROSETTA/main/source/bin/AbinitioRelax.linuxgccrelease **@options.txt**

```
-in:file
      -fasta ./input_files/1e1wA.fasta
      -native ./input_files/1e1w.pdb
      -frag3 ./input_files/aa1elwA03_05.200_v1_3
      -frag9 ./input_files/aa1elwA09_05.200_v1_3
-psipred_ss2 ./input_files/1elwA.psipred_ss2
-abinitio:relax
-relax:fast
-abinitio::increase_cycles 10
-abinitio::rg_reweight 0.5
…
-out:file:silent ./output_files/1elwA_silent.out
-nstruct 10
```

Applications



Applications (old school)

.../main/source/bin/**<app_name>**.default.linuxgccrelease

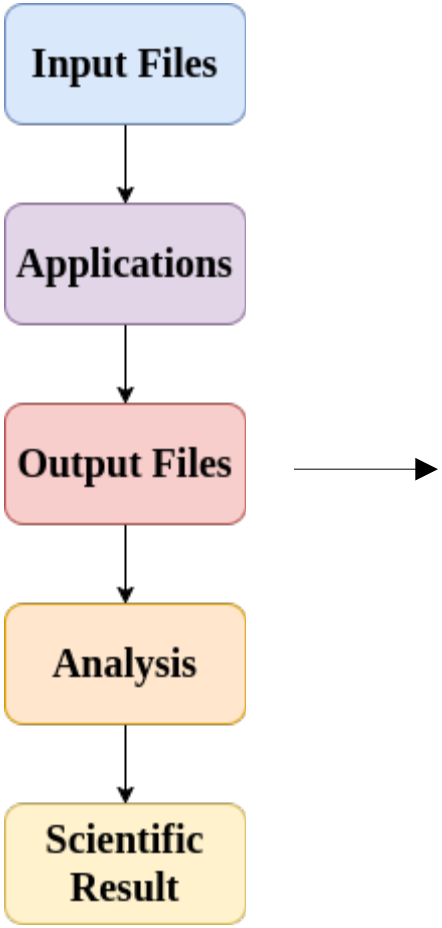
AbinitioRelax
docking_protocol
Fixbb
antibody_designer

Movers/XML files (default)

.../main/source/bin/**rosetta_scripts**.default.linuxgccrelease \
-parser:protocol XXX.xml

DockingProtocolMover
FixBBMover
FastDesignMover

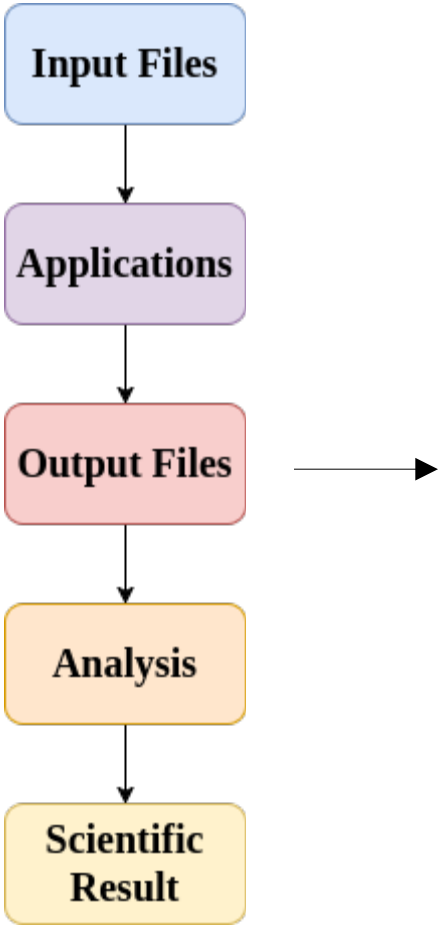
Output Files



Structures: PDB files
- International standard
- Readable by Pymol, MOE, Chimera, etc
- One line per atom
- Useful for small number of structures

Structures: Silent files
- Specific to Rosetta
- Compact
- One line per residue
- Useful for archiving
- Also possible in binary silent files (non readable by humans)

Output Files



Score file (score.sc)

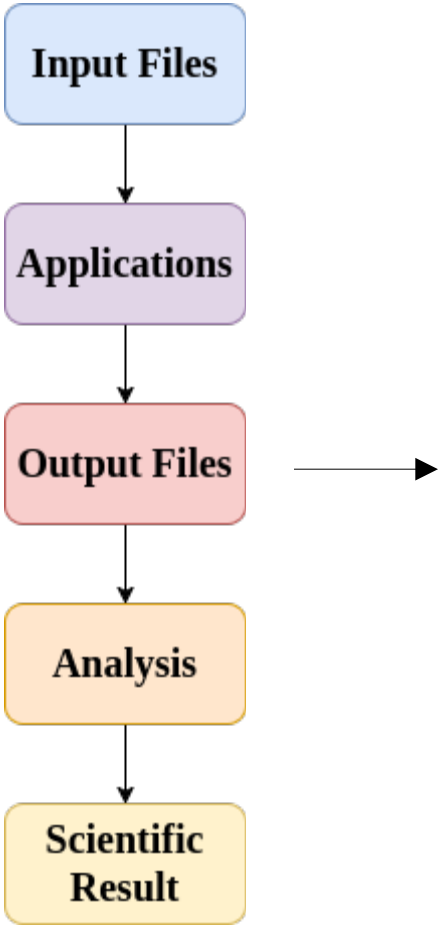
- One output model per line
- Second column is “Total score”
- Last column is the output model name
- Each column in between is a score term

```
SEQUENCE:
SCORE:     score     fa_atr     fa_rep     fa_sol    fa_intra_rep    fa_elec    ...
SCORE:  -1217.209  -2778.696    266.309   1545.149           5.900   -301.320   ...
SCORE:  -1217.028  -2792.422    263.906   1549.738           5.867   -295.799   ...
SCORE:  -1204.280  -2760.354    259.175   1534.072           5.913   -293.050   ...
SCORE:  -1207.127  -2768.191    260.443   1541.857           5.881   -301.847   ...
SCORE:  -1208.390  -2769.872    262.398   1539.668           5.879   -297.571   ...
```

Score (in pdb file)

```
ATOM   3381 2HG2 THR L 227     -35.593  22.831  31.238  1.00  0.00           H
ATOM   3382 3HG2 THR L 227     -34.799  21.240  31.213  1.00  0.00           H
TER
# All scores below are weighted scores, not raw scores.
#BEGIN_POSE_ENERGIES_TABLE 3gbn_Ab_0005.pdb
label fa_atr fa_rep fa_sol fa_intra_rep fa_elec pro_close hbond_sr_bb hbond_lr_bb hbc
weights 1 0.55 0.9375 0.005 0.875 1.25 1.17 1.17 1.17 1.1 1.25 0.25 0.625 0.7 0.4 0.6
pose -994.338 137.719 561.027 2.15688 -112.612 19.7634 -12.2069 -79.5391 -24.1449 -23
GLU:NtermProteinFull_1 -1.58225 0.53996 1.45283 0.00353 0.06909 0 0 0 0 0 0 0 0.01109
VAL 2 -3.34255 0.45648 1.46378 0.01322 -0.08167 0 0 0 0 0 0 -0.16095 0.87346 0.30715
```

Output Files



Tracer output (Log file)
- Report your command at the beginning
- Reports databases, protocols, errors
- Useful for debugging
- Makes your protocol reproducible
- Take a bunch of space!

Options to control tracer output:
- Silence certain tracers:
  mute core.chemical.ResidueTypeSet
- Change verbosity level
  (Error/Warning/Info/Debug/Trace)
  out:levels all:Warning core.init:Info

Resources for Users:

https://www.rosettacommons.org

Documentation
User guides
Forum
Software Download
Tutorials
(https://meilerlab.org/tutorials/)

Us teachers at this workshop (email us whenever, we do answer!)