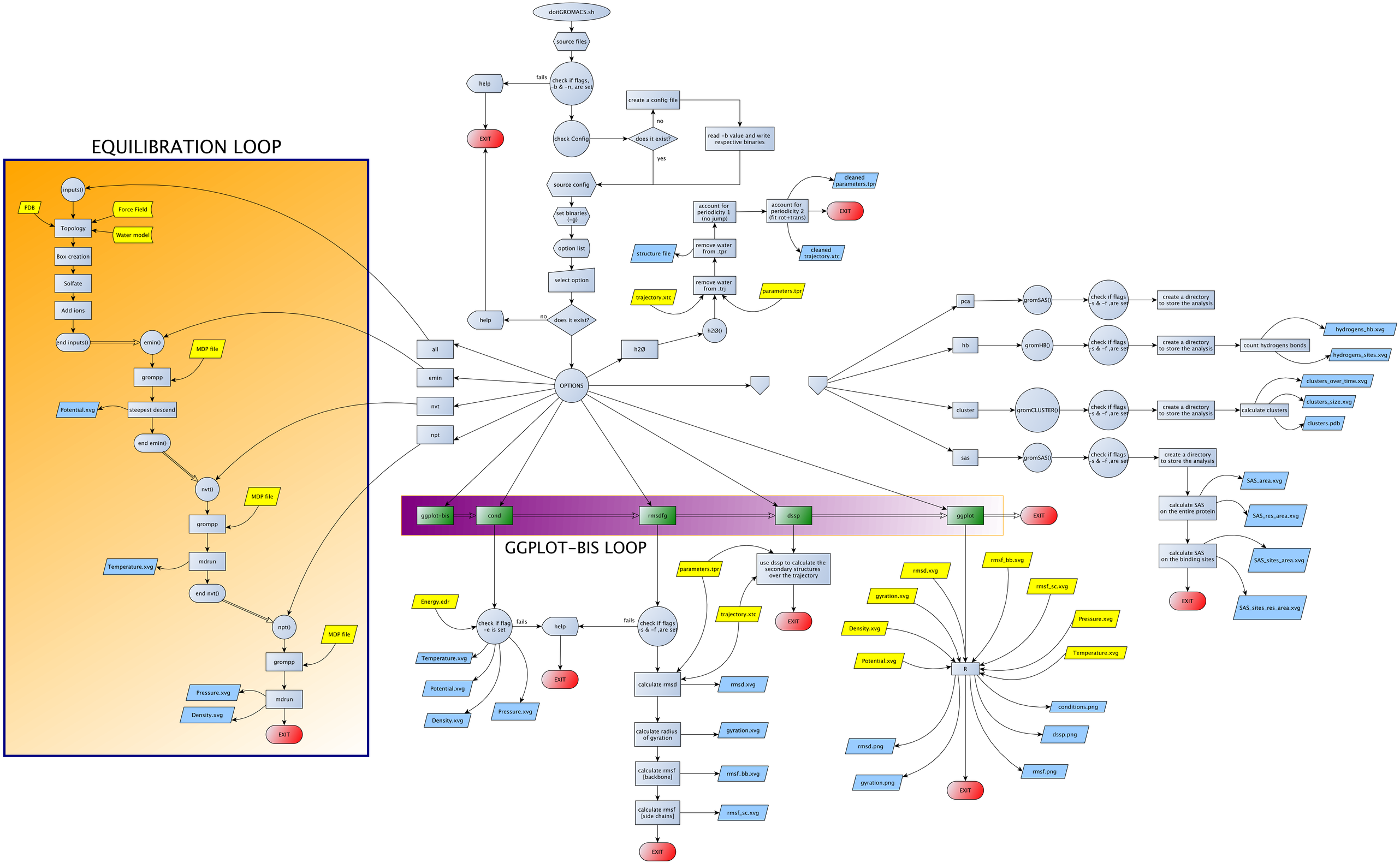
EQUILIBRATION LOOP
inputs()
PDB
Force Field
Topology
Water model
Box creation
Solfate
Add ions
end inputs()
emin()
MDP file
grompp
Potential.xvg
steepest descend
end emin()
nvt()
MDP file
grompp
Temperature.xvg
mdrun
end nvt()
npt()
MDP file
grompp
Pressure.xvg
Density.xvg
mdrun
EXIT
doitGROMACS.sh
source files
fails
help
check if flags, -b & -n, are set
EXIT
check Config
does it exist?
no
create a config file
yes
read -b value and write respective binaries
source config
set binaries (-g)
option list
select option
no
help
does it exist?
OPTIONS
all
emin
nvt
npt
h2Ø
h2Ø()
remove water from .trj
trajectory.xtc
parameters.tpr
remove water from .tpr
structure file
account for periodicity 1 (no jump)
account for periodicity 2 (fit rot+trans)
EXIT
cleaned parameters.tpr
cleaned trajectory.xtc
GGPLOT-BIS LOOP
ggplot-bis
cond
rmsdfg
dssp
ggplot
EXIT
Energy.edr
check if flag -e is set
fails
help
EXIT
Temperature.xvg
Potential.xvg
Density.xvg
Pressure.xvg
fails
check if flags -s & -f ,are set
calculate rmsd
rmsd.xvg
calculate radius of gyration
gyration.xvg
calculate rmsf [backbone]
rmsf_bb.xvg
calculate rmsf [side chains]
rmsf_sc.xvg
EXIT
parameters.tpr
trajectory.xtc
use dssp to calculate the secondary structures over the trajectory
EXIT
rmsd.xvg
gyration.xvg
Density.xvg
Potential.xvg
rmsf_bb.xvg
rmsf_sc.xvg
Pressure.xvg
Temperature.xvg
R
conditions.png
dssp.png
rmsf.png
rmsd.png
gyration.png
EXIT
pca
gromSAS()
check if flags -s & -f ,are set
create a directory to store the analysis
hb
gromHB()
check if flags -s & -f ,are set
create a directory to store the analysis
count hydrogens bonds
hydrogens_hb.xvg
hydrogens_sites.xvg
cluster
gromCLUSTER()
check if flags -s & -f ,are set
create a directory to store the analysis
calculate clusters
clusters_over_time.xvg
clusters_size.xvg
clusters.pdb
sas
gromSAS()
check if flags -s & -f ,are set
create a directory to store the analysis
calculate SAS on the entire protein
SAS_area.xvg
SAS_res_area.xvg
calculate SAS on the binding sites
SAS_sites_area.xvg
SAS_sites_res_area.xvg
EXIT