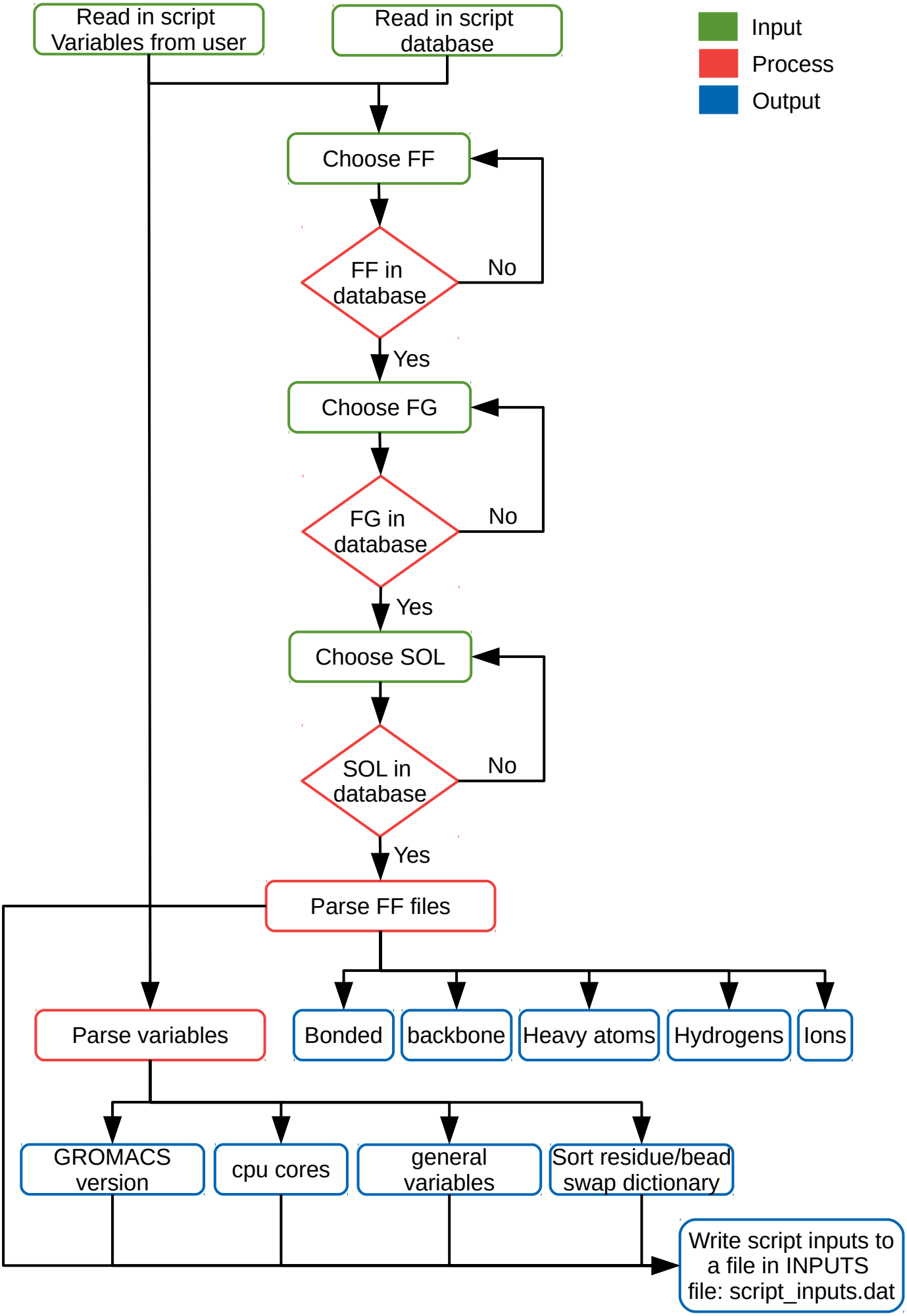
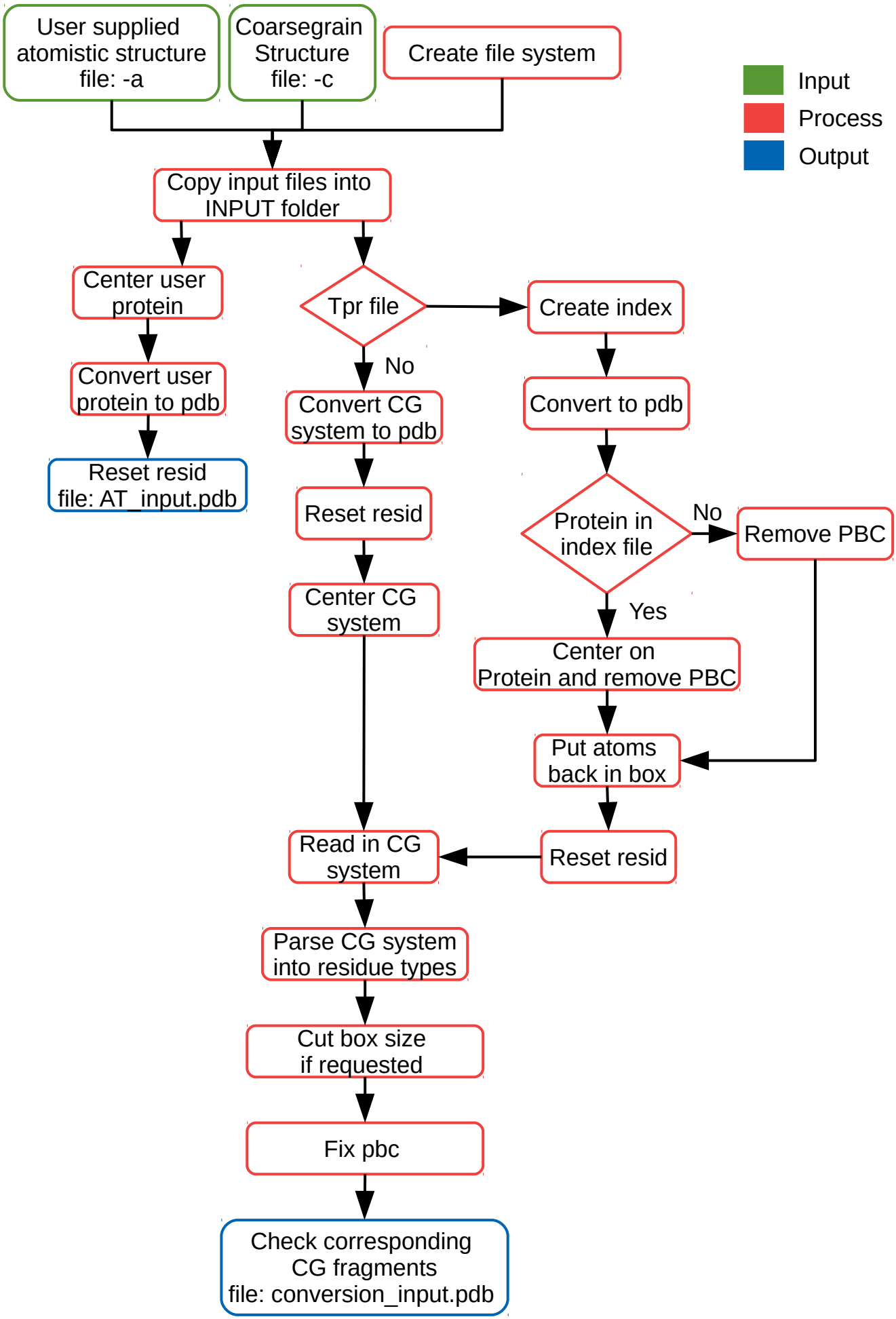
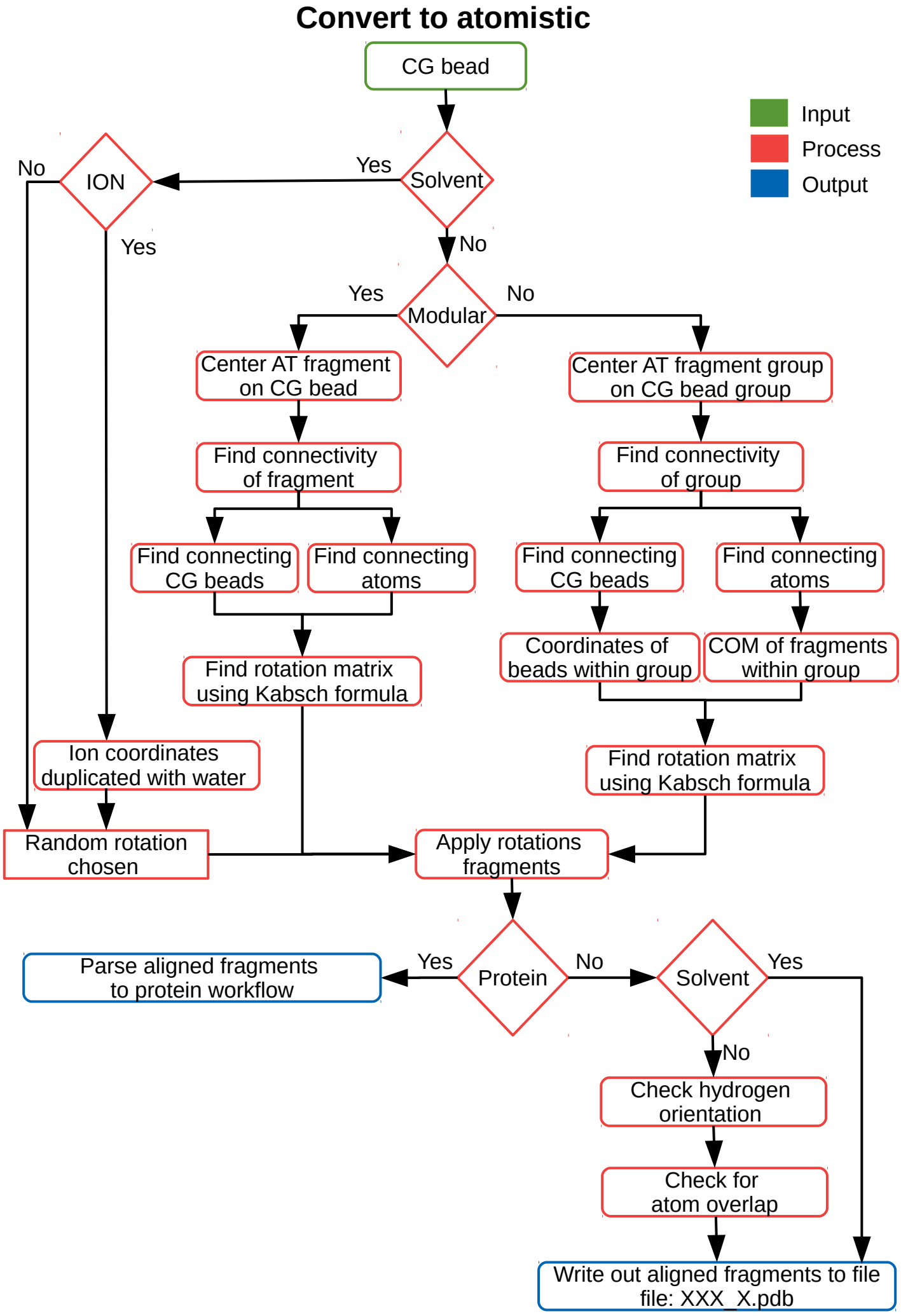
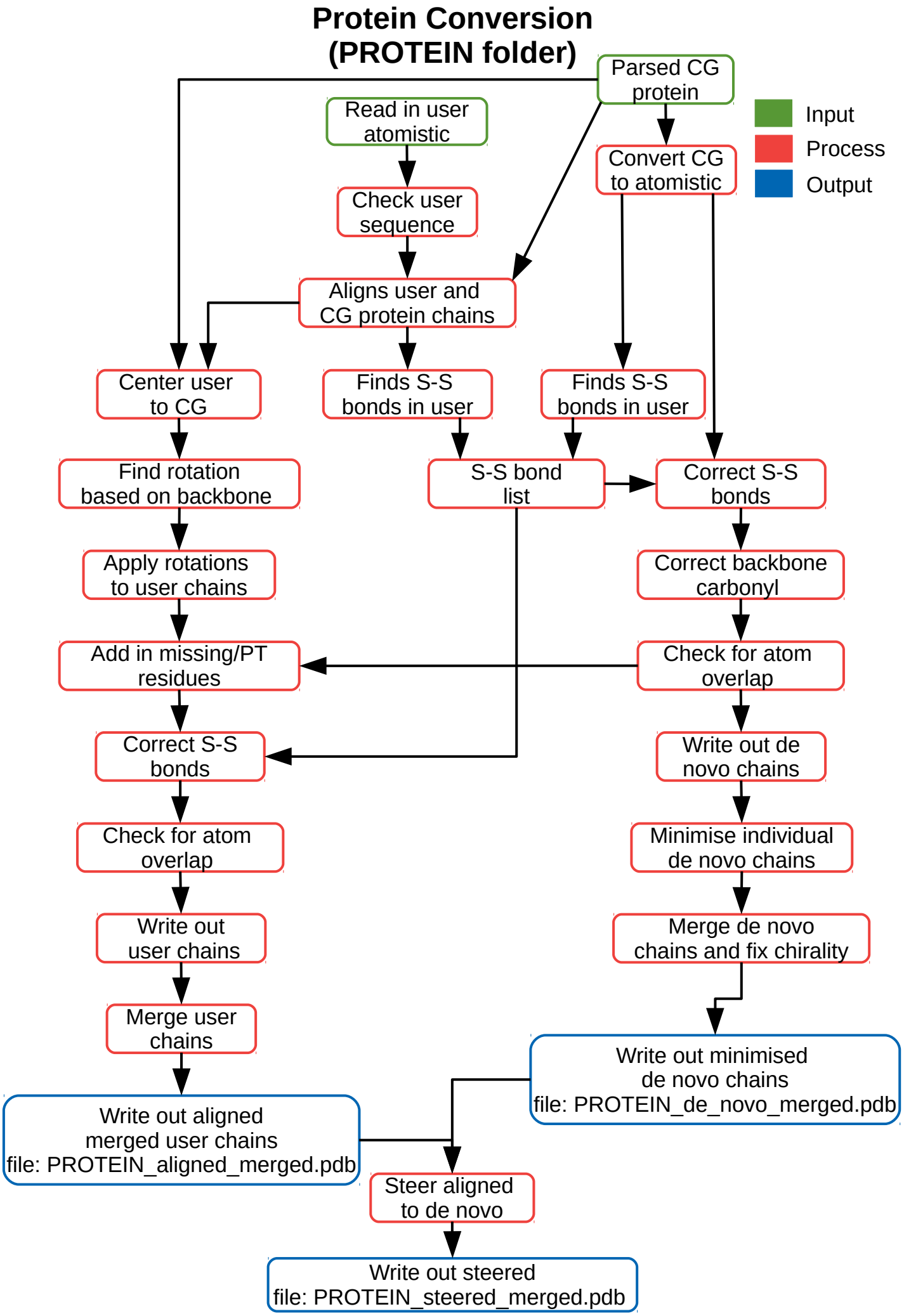
Initialisation



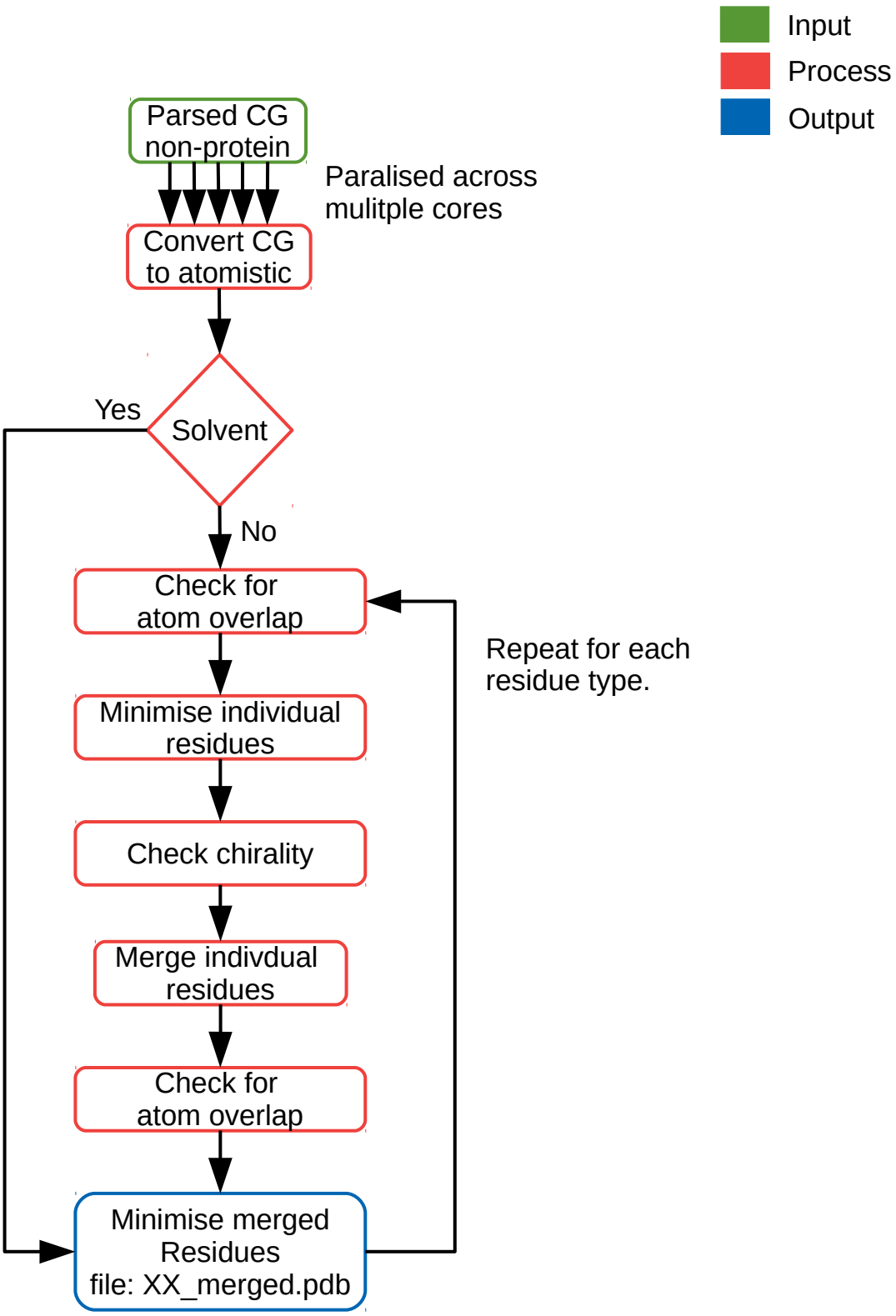
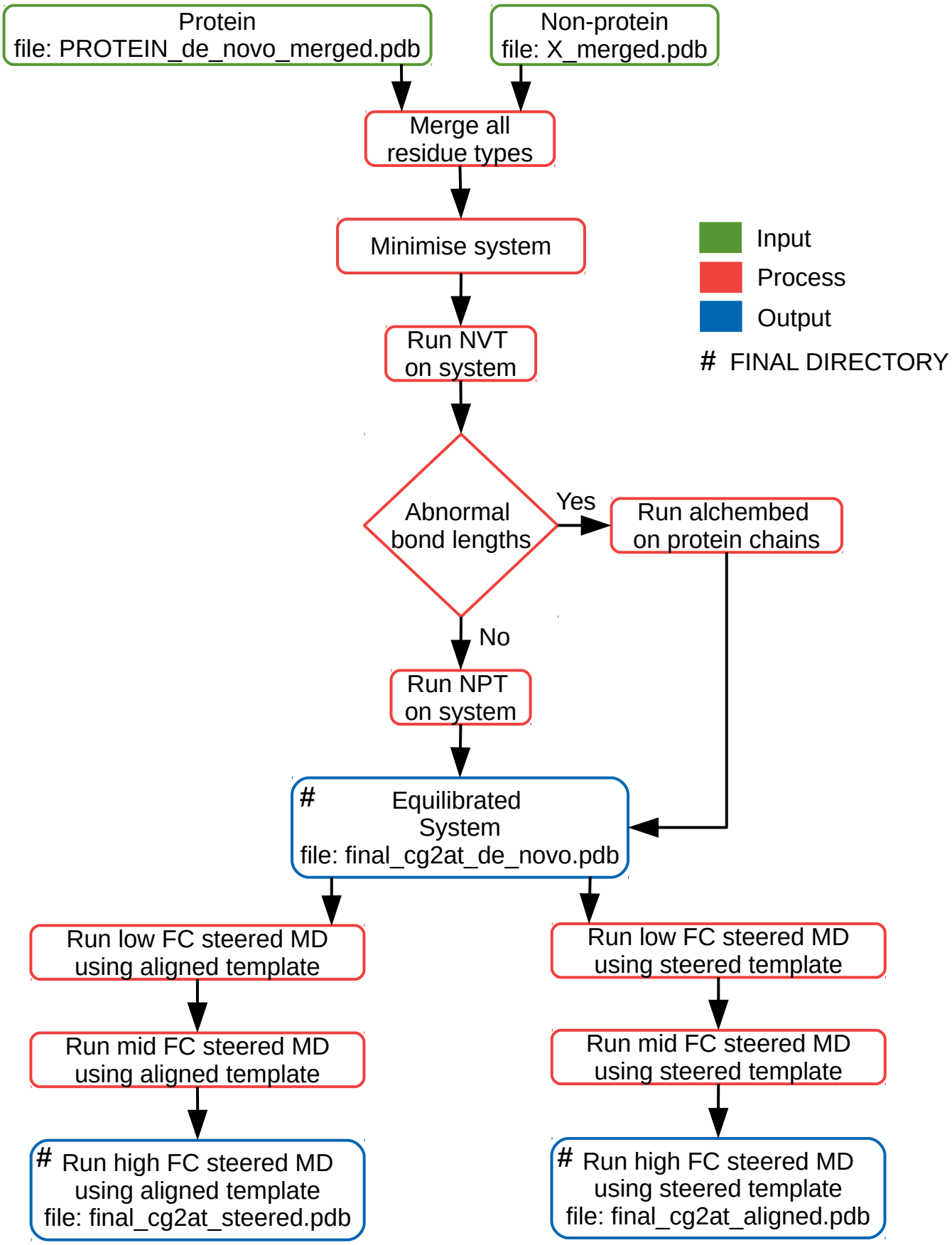
System setup
(INPUTS folder)




Convert to atomistic
CG bead
Input
Process
Output
Solvent
Yes
ION
No
Yes
No
Modular
Yes
No
Center AT fragment on CG bead
Center AT fragment group on CG bead group
Find connectivity of fragment
Find connectivity of group
Find connecting CG beads
Find connecting atoms
Find connecting CG beads
Find connecting atoms
Find rotation matrix using Kabsch formula
Coordinates of beads within group
COM of fragments within group
Ion coordinates duplicated with water
Find rotation matrix using Kabsch formula
Random rotation chosen
Apply rotations fragments
Parse aligned fragments to protein workflow
Yes
Protein
No
Solvent
Yes
No
Check hydrogen orientation
Check for atom overlap
Write out aligned fragments to file file: XXX_X.pdb


Protein Conversion
(PROTEIN folder)
Parsed CG protein
Read in user atomistic
Convert CG to atomistic
Check user sequence
Aligns user and CG protein chains
Center user to CG
Finds S-S bonds in user
Finds S-S bonds in user
Find rotation based on backbone
S-S bond list
Correct S-S bonds
Apply rotations to user chains
Correct backbone carbonyl
Add in missing/PT residues
Check for atom overlap
Correct S-S bonds
Write out de novo chains
Check for atom overlap
Minimise individual de novo chains
Write out user chains
Merge de novo chains and fix chirality
Merge user chains
Write out minimised de novo chains
file: PROTEIN_de_novo_merged.pdb
Write out aligned merged user chains
file: PROTEIN_aligned_merged.pdb
Steer aligned to de novo
Write out steered
file: PROTEIN_steered_merged.pdb
Input
Process
Output

Non-Protein Conversion
(POPG, POPE, SOL etc folders)



System build
(MERGED folder)