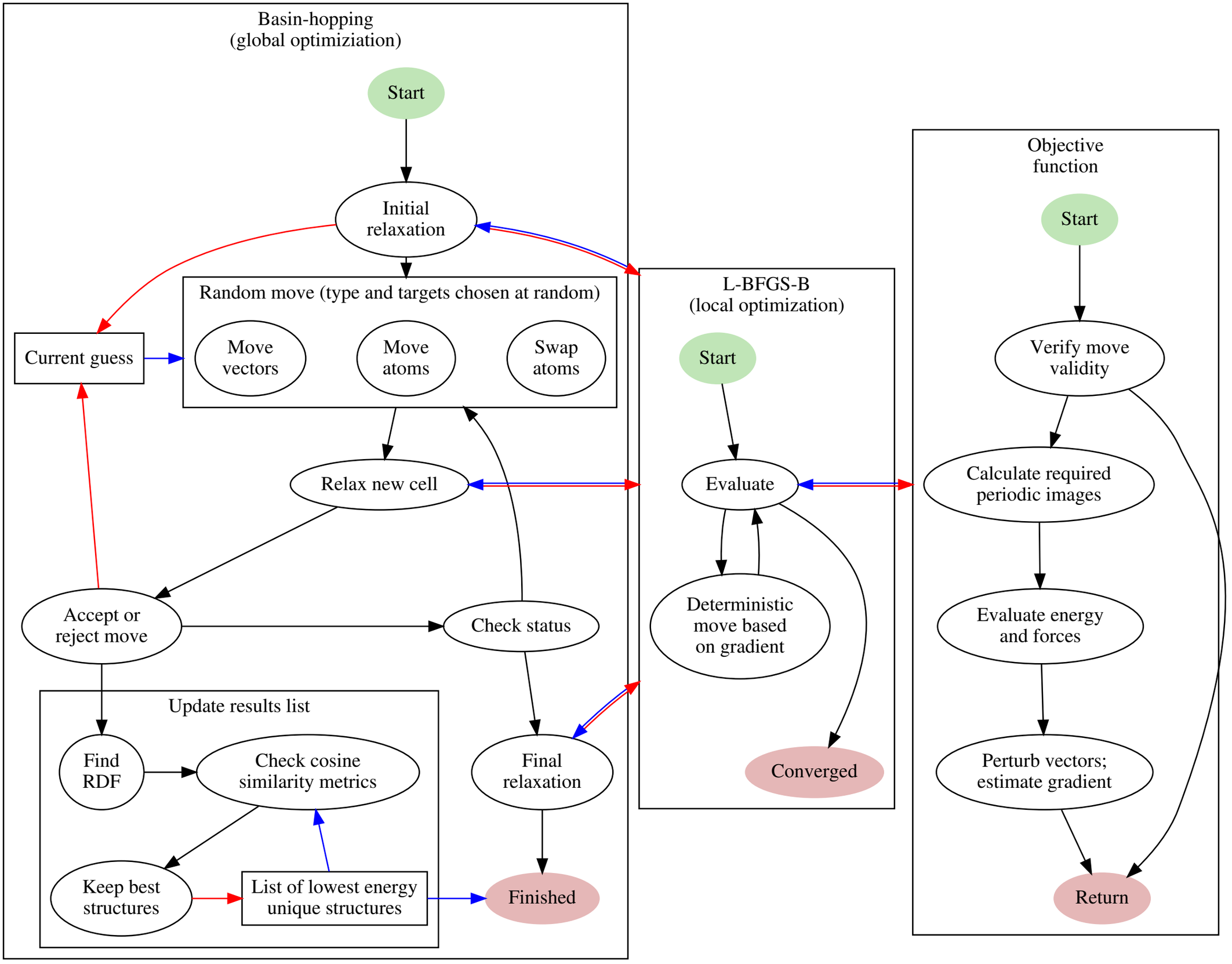
Basin-hopping
(global optimiziation)
Start
Initial relaxation
Random move (type and targets chosen at random)
Current guess
Move vectors
Move atoms
Swap atoms
Relax new cell
Accept or reject move
Check status
Update results list
Find RDF
Check cosine similarity metrics
Keep best structures
List of lowest energy unique structures
Final relaxation
Finished
L-BFGS-B
(local optimization)
Start
Evaluate
Deterministic move based on gradient
Converged
Objective function
Start
Verify move validity
Calculate required periodic images
Evaluate energy and forces
Perturb vectors; estimate gradient
Return