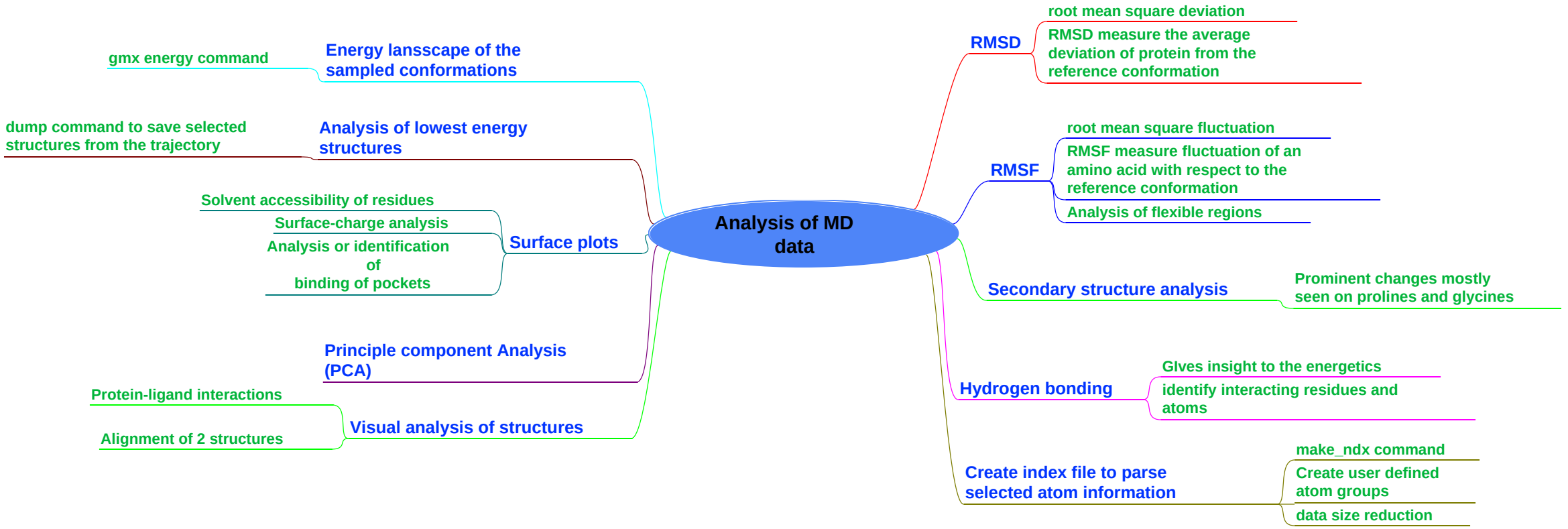
Analysis of MD data
Energy lansscape of the sampled conformations
gmx energy command
Analysis of lowest energy structures
dump command to save selected structures from the trajectory
Surface plots
Solvent accessibility of residues
Surface-charge analysis
Analysis or identification of binding of pockets
Principle component Analysis (PCA)
Visual analysis of structures
Protein-ligand interactions
Alignment of 2 structures
RMSD
root mean square deviation
RMSD measure the average deviation of protein from the reference conformation
RMSF
root mean square fluctuation
RMSF measure fluctuation of an amino acid with respect to the reference conformation
Analysis of flexible regions
Secondary structure analysis
Prominent changes mostly seen on prolines and glycines
Hydrogen bonding
GIves insight to the energetics
identify interacting residues and atoms
Create index file to parse selected atom information
make_ndx command
Create user defined atom groups
data size reduction