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## *List of Abbreviations*

3D	3 Dimensional
AMBER	Assisted Model Building with Energy Refinement
AMPs	Antimicrobial Peptides
ARG	Arginine
ASP	Asparagine
DNA	Deoxyribonucleic Acid
DSSP	Dictionary of protein secondary structure
FS	Femto Second
GB	Generalized Born
GBSA	Generalized Born Surface Area
GLN	Glutamine
GLU	Glutamic Acid
GROMACS	GRONingen MACHine for Chemical Simulations
HB	Hydrogen Bond
ILE	Isoleucine
K	Kelvin
K CAL / MOL	Kilo Calorie per mole
LEU	Leucine
LYS	Lysine
M	Molar
MC	Monte Carlo
MD	Molecular Dynamics
MM	<i>Molecular Mechanics</i>
NMR	Nuclear Magnetic Resonance
NS	Nano Second
OBC	Onufriev, Bashford and Case

PBC	Periodic Boundary Conditions
PDB	Protein Data Bank
PHE	Phenylalanine
PS	Pico Second
PTRAJ	Process Trajectory
RCSB	The Research Collaboratory for Structural Bioinformatics
RMSD	Root Mean Square Deviation
SANDER	Simulated Annealing with NMR-Derived Energy Restraints
SASA	Solvent Accessible Surface Area
SPC	Simple point charge
VMD	Visual Molecular Dynamics