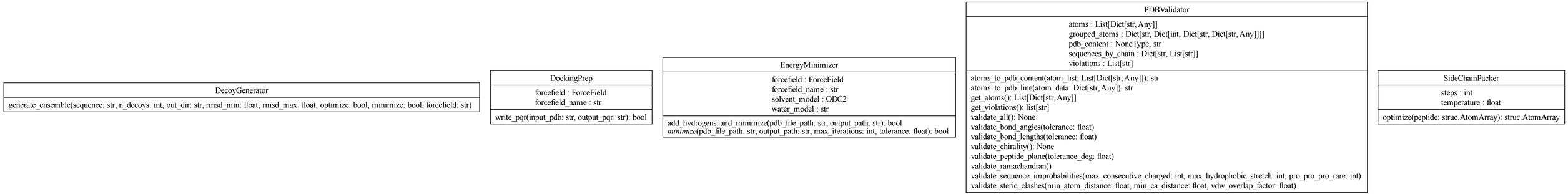
DecoyGenerator
generate_ensemble(sequence: str, n_decoys: int, out_dir: str, rmsd_min: float, rmsd_max: float, optimize: bool, minimize: bool, forcefield: str)
DockingPrep
forcefield : ForceField
forcefield_name : str
write_pqr(input_pdb: str, output_pqr: str): bool
EnergyMinimizer
forcefield : ForceField
forcefield_name : str
solvent_model : OBC2
water_model : str
add_hydrogens_and_minimize(pdb_file_path: str, output_path: str): bool
minimize(pdb_file_path: str, output_path: str, max_iterations: int, tolerance: float): bool
PDBValidator
atoms : List[Dict[str, Any]]
grouped_atoms : Dict[str, Dict[int, Dict[str, Dict[str, Any]]]]
pdb_content : NoneType, str
sequences_by_chain : Dict[str, List[str]]
violations : List[str]
atoms_to_pdb_content(atom_list: List[Dict[str, Any]]): str
atoms_to_pdb_line(atom_data: Dict[str, Any]): str
get_atoms(): List[Dict[str, Any]]
get_violations(): list[str]
validate_all(): None
validate_bond_angles(tolerance: float)
validate_bond_lengths(tolerance: float)
validate_chirality(): None
validate_peptide_plane(tolerance_deg: float)
validate_ramachandran()
validate_sequence_improbabilities(max_consecutive_charged: int, max_hydrophobic_stretch: int, pro_pro_pro_rare: int)
validate_steric_clashes(min_atom_distance: float, min_ca_distance: float, vdw_overlap_factor: float)
SideChainPacker
steps : int
temperature : float
optimize(peptide: struc.AtomArray): struc.AtomArray