

DatasetGenerator
max_length : int min_length : int num_samples : int output_dir : Path train_ratio : float
generate() prepare_directories()

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 : NoneType, OBC2 water_model : str
add_hydrogens_and_minimize(pdb_file_path, output_path) equilibrate(pdb_file_path, output_path, steps) minimize(pdb_file_path, output_path, max_iterations, tolerance)

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