

GEM-PRO descriptor	Description
ovality	(SASA/Nres <sup>2/3</sup> )
ssb_avg_res_depth	average angstrom distance to surface (averaged over all atoms in residue)
ssb_ca_depth	average angstrom distance to surface (averaged over all alpha carbon atoms in residue)
ssb_cys_bridge	number of cysteine bridges
ssb_mean_rel_exposed	relative mean exposed surface area
ssb_per_310_helix	percent 310 helical residues in protein
ssb_per_5_helix	percent pi helical residues in protein
ssb_per_B	percent of buried residues in protein
ssb_per_B_NP	percent of buried nonpolar residues in protein
ssb_per_B_P	percent of buried polar residues in protein
ssb_per_B_neg	percent of buried negative residues in protein
ssb_per_B_pos	percent of buried positive residues in protein
ssb_per_NP	percent nonpolar residues in protein
ssb_per_P	percent polar residues in protein
ssb_per_S	percent of surface residues in protein
ssb_per_S_NP	percent of surface nonpolar residues in protein
ssb_per_S_P	percent of surface polar residues in protein
ssb_per_S_neg	percent of surface negative residues in protein
ssb_per_S_pos	percent of surface positive residues in protein
ssb_per_alpha	percent alpha helical residues in protein
ssb_per_bent	percent bent/coil residues in protein
ssb_per_beta_bridge	percent beta bridge residues in protein
ssb_per_ext_beta	percent beta sheet residues in protein
ssb_per_hbond_turn	percent residues participating in hydrogen bonds at turns in protein
ssb_per_irr	percent disordered residues in protein
ssb_per_neg	percent negative residues in protein
ssb_per_pos	percent positive residues in protein
ssb_sasa	solvent exposed surface area
ssb_size	total size (amino acid length)

Table S5: The GEM-PRO columns corresponding to computed structural properties and their descriptions.