calc_xscore::txring + valid + ttype + num_member + atom_id + atom_count + atom_max + bond_id + bond_count

+ bond max

+ centroid

calc_xscore::txbond + id + valid + atom_1 + atom_2 + ttype + part

+ ring

+ neib

+ length

+ num neib

calc_xscore::txatom + topindex + id + valid + mask + name + ttype + xtype + xtype + type2 + residue + old_residue and 25 more...

