

calc_xscore::txatom

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

+atom_1
+atom_2
+atom_3
+atom_4



calc_xscore::txtorsion

+ ttype
+ angle
+ v
+ n
+ s
+ e