calc_xscore::txatom

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

+a
+d
+h

calc_xscore::txhbond

+ valid
+ ttype
+ d_type
+ a_type
+ sb
+ latom
+ patom
+ dd
+ a0
+ a1
+ a2
+ score