Supplementary Figure 1

Flow chart of steps in producing the TSH-TSHR LRD structure based on the 2.9 Å structure of the FSH-FSHR LRD (Fan & Hendrickson 2005) and the 2.55 Å crystal structure of the M22-TSHR LRD (Sanders et al. 2007a).
Crystal structure of the FSH-FSHR LRD complex

FUGUE

FSH-FSHR LRD and TSH-TSHR LRD amino acid sequence alignment

Preliminary model of the TSH-TSHR LRD structure

MODELLER

Manual realignment

PROCHECK, Verify3D and JOY validation programs

TSHR LRD in the model replaced by TSHR LRD crystal structure

Crystal structure of M22-TSHR LRD and TSH-TSHR LRD coordinates superimposed

First model of the structure of the TSH-TSHR LRD complex

Interface optimization

Final structure of the TSH-TSHR LRD complex

Good validation parameters?

YES

NO