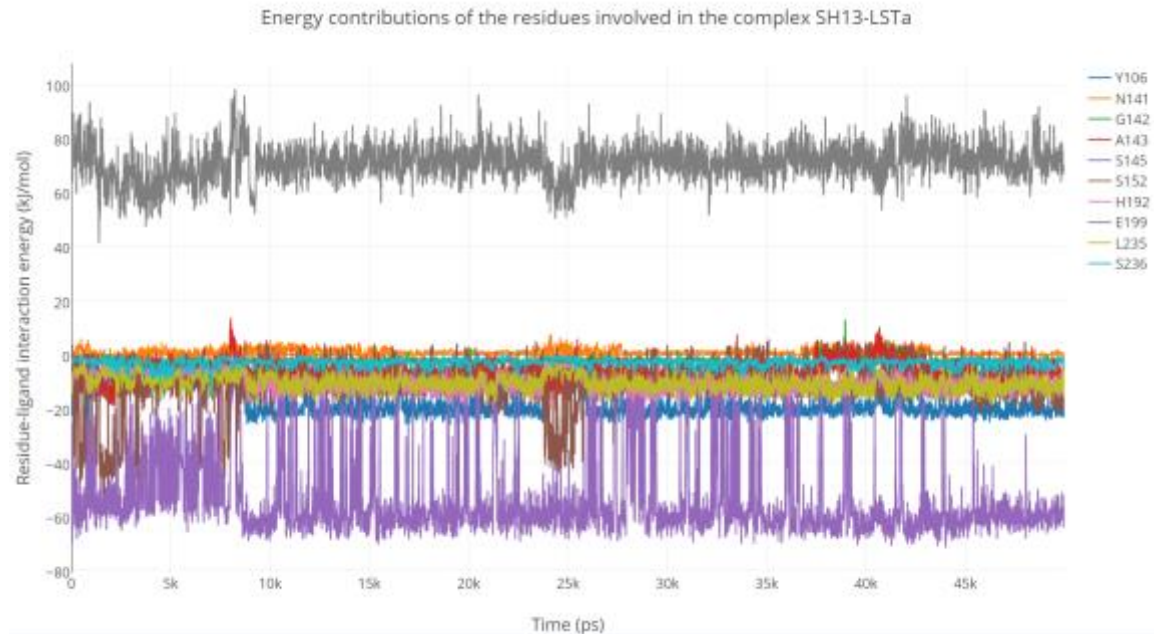


Additional file 5. Residue contributions during the whole simulation process.

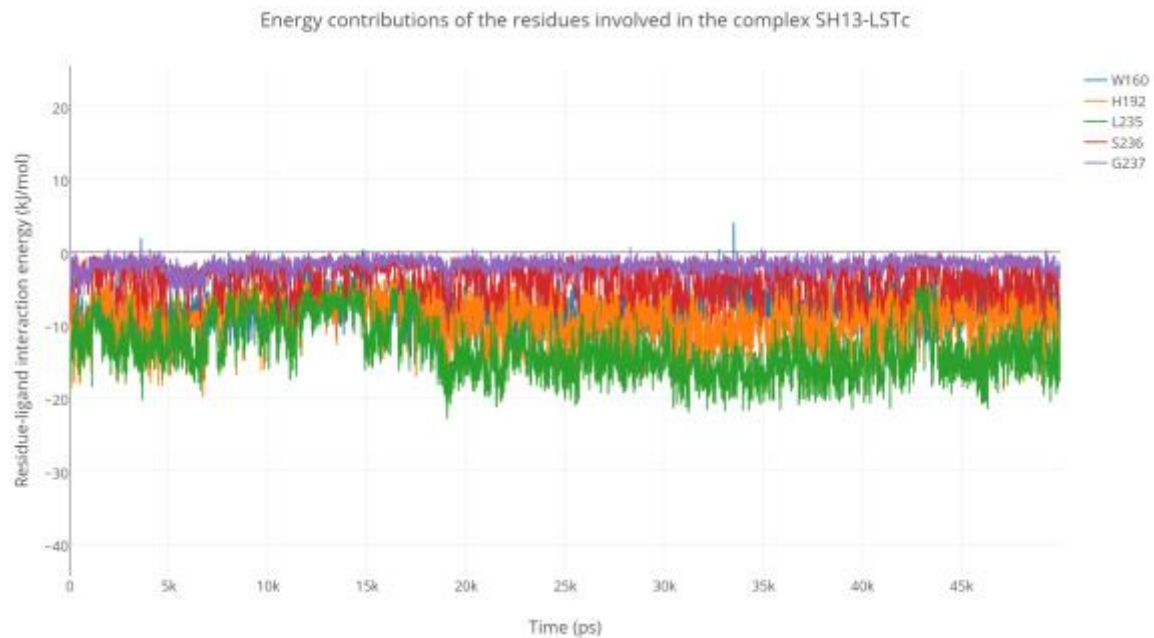
1. Energy contribution of the residues involved in interaction in the complex SH13-LSTa

For most residues, the residue-ligand interaction energy fluctuated within a small range, except S145 and S152.



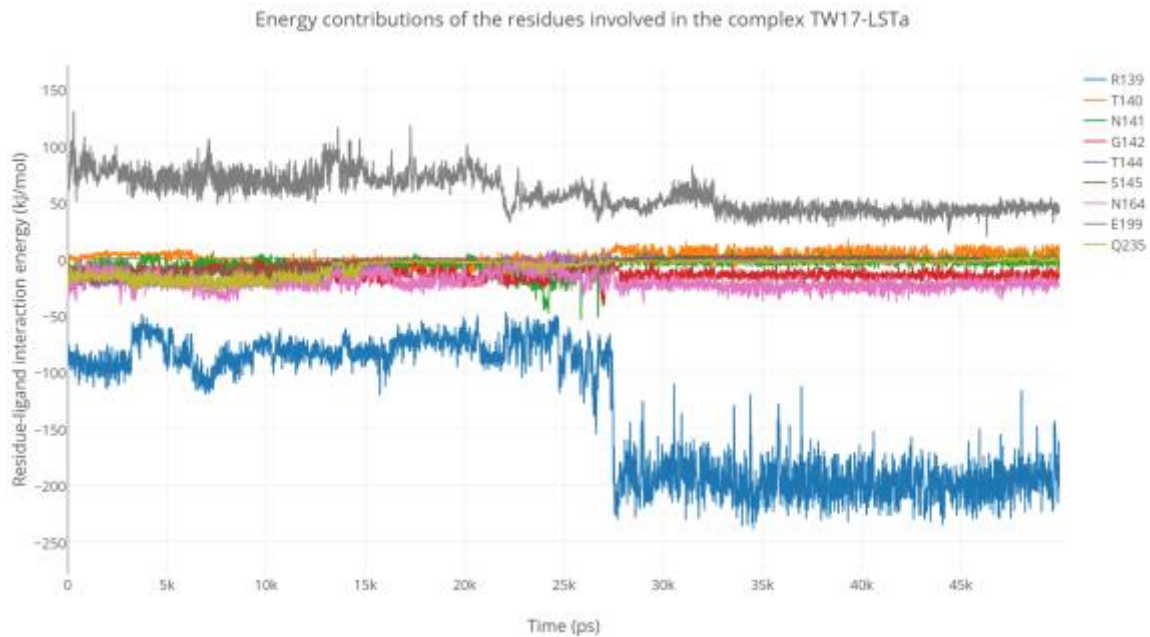
2. Energy contribution of the residues involved in interaction in the complex SH13-LSTc.

The residue-ligand interaction energy fluctuated within 10 kJ/mol after 20 ns.



3. Energy contribution of the residues involved in interaction in the complex TW17-LSTa.

For most residues, the residue-ligand interaction energy fluctuated within a small range for the whole simulation process, except R139, which converged after 28 ns.



4. Energy contribution of the residues involved in interaction in the complex TW17-LSTc.

The residue-ligand interaction energy fluctuated within a small range. The fluctuation for R139 is slightly larger than the others.

