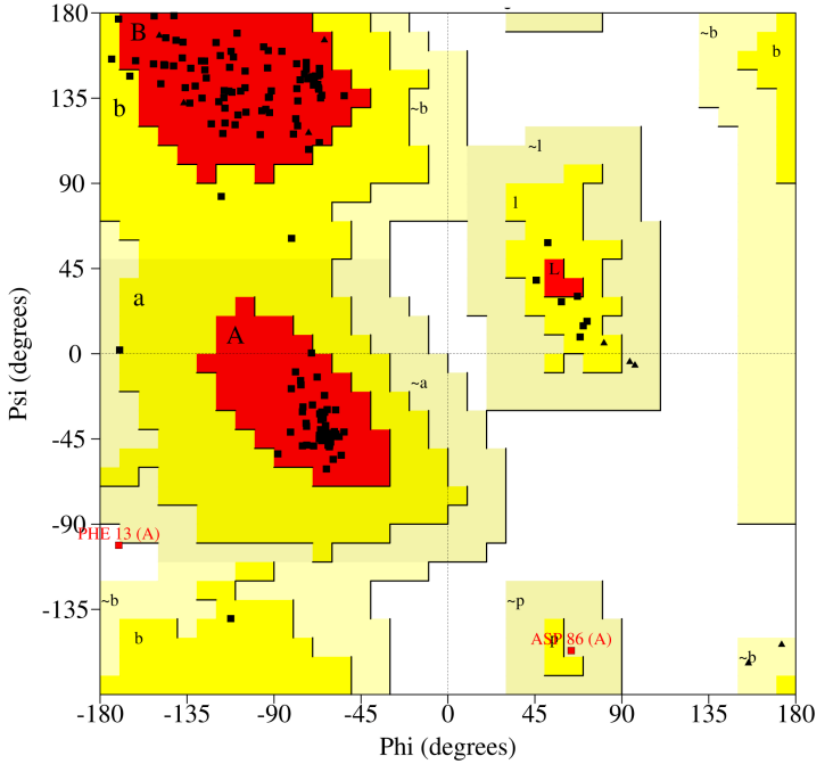
1A

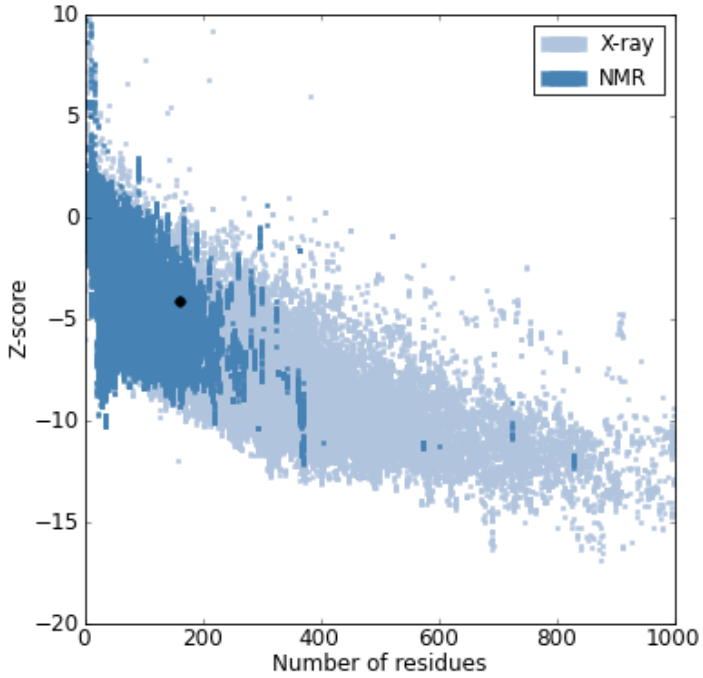


Plot statistics

Residues in most favoured regions [A,B,L]	122	89.1%
Residues in additional allowed regions [a,b,l,p]	13	9.5%
Residues in generously allowed regions [~a,~b,~l,~p]	1	0.7%
Residues in disallowed regions	1	0.7%
Number of non-glycine and non-proline residues	137	100.0%
Number of end-residues (excl. Gly and Pro)	2	
Number of glycine residues (shown as triangles)	9	
Number of proline residues	13	
Total number of residues	161	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

1B

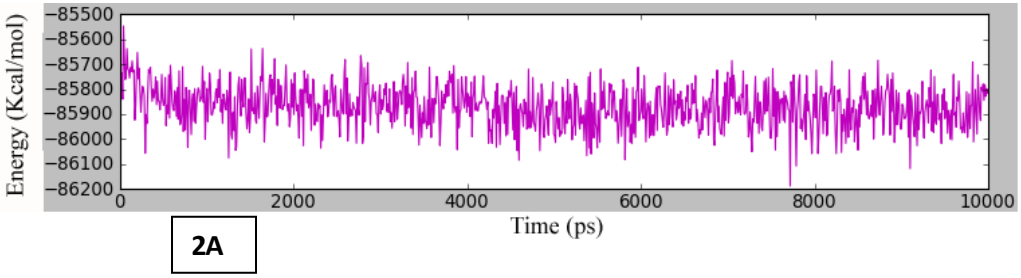


Supplementary Figure 1: Validation of AccB homology model

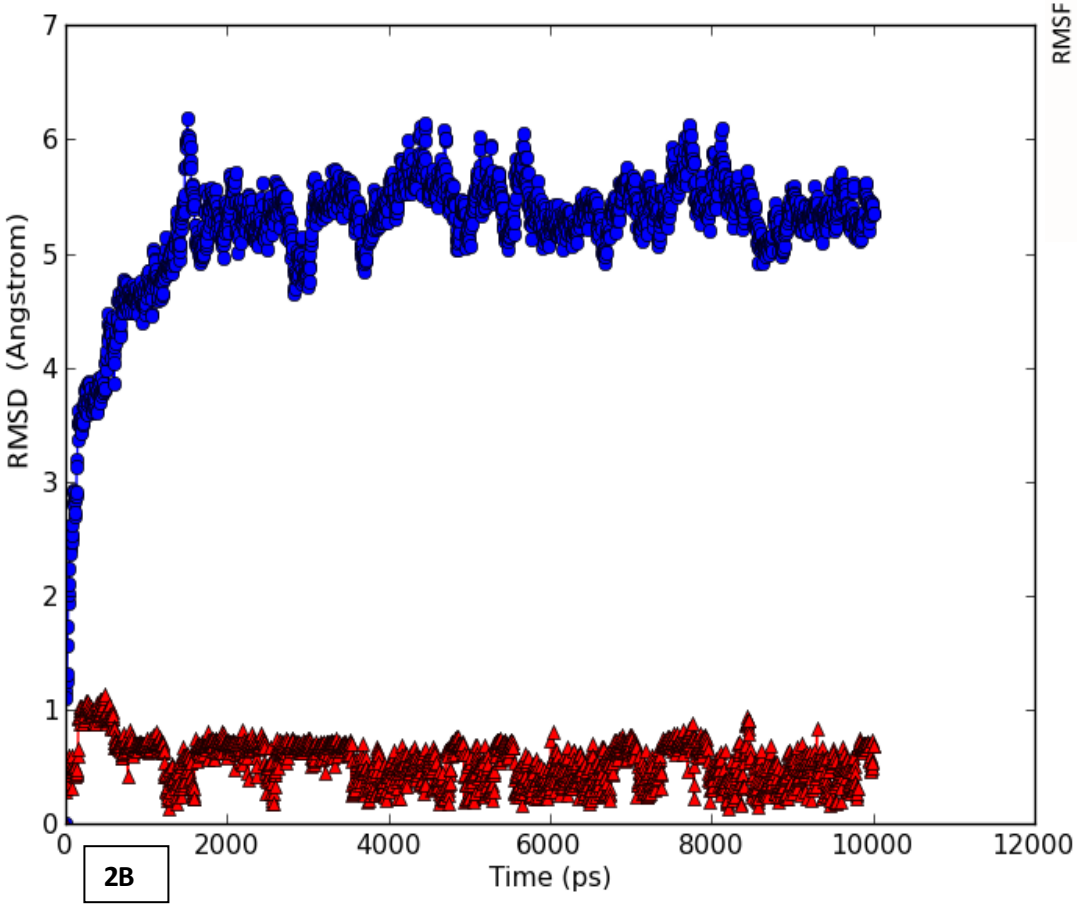
A) PROCHECK analysis

B) B) ProSA analysis

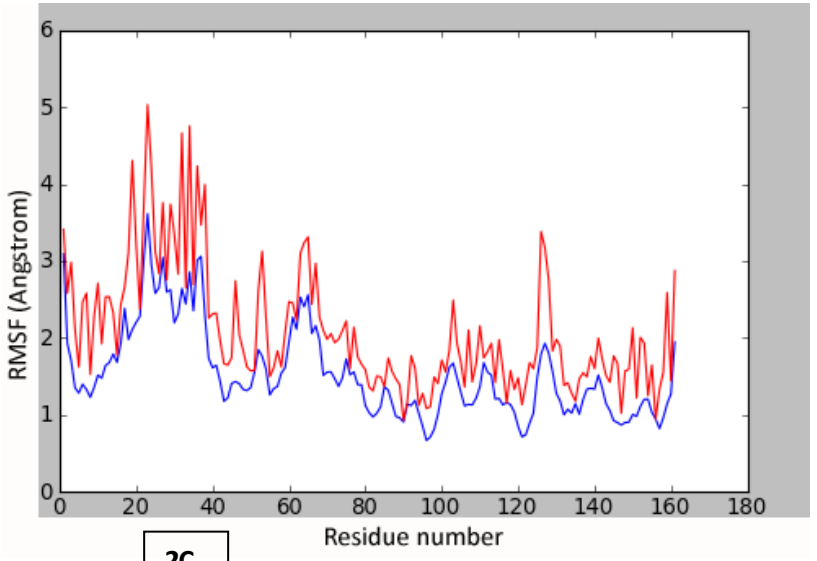
AccB = Biotin carboxyl carrier protein of acetyl-CoA carboxylase



2A



2B



2C

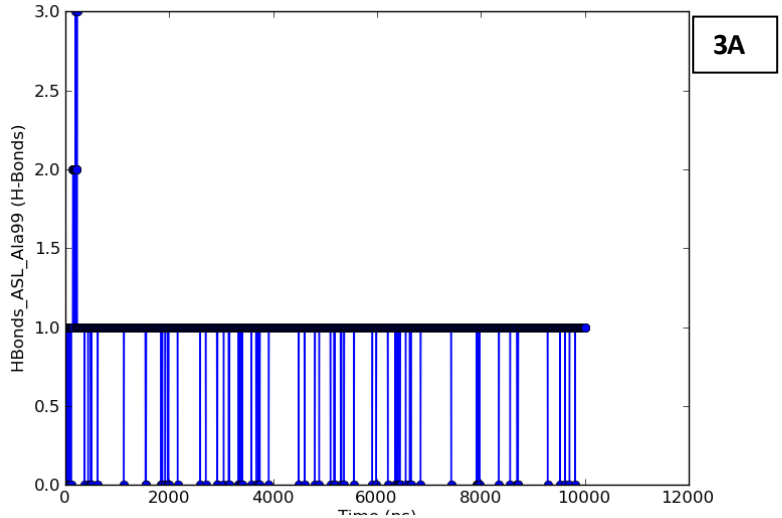
Supplementary Figure 2: Interactions of AccB with lead1 after 10ns Molecular dynamics simulations

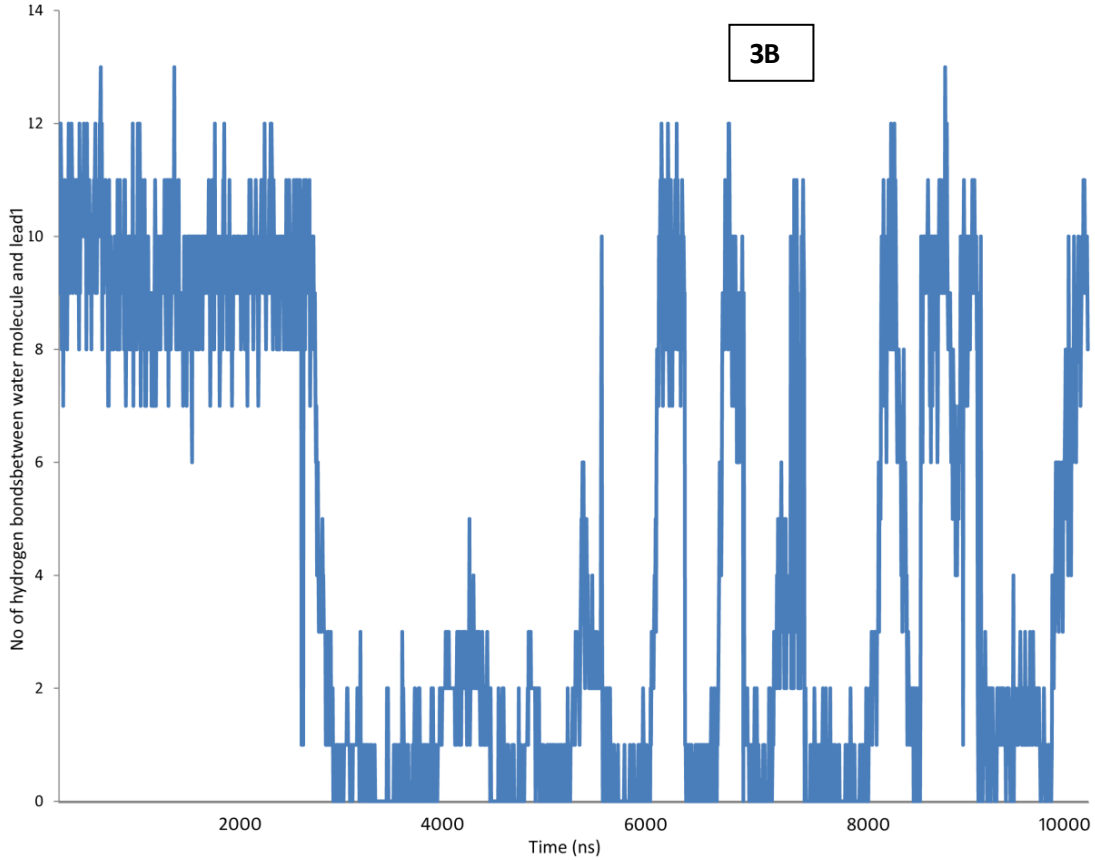
A) Energy plot

B) RMSD plot

C) RMSF plot

AccB = Biotin carboxyl carrier protein of acetyl-CoA carboxylase RMSD = Root mean square deviation; RMSF = Root mean square fluctuation





Supplementary Figure 3: Hydrogen bond monitoring in all 2084 trajectories. A) Hydrogen bond interactions between Ala 99 and lead1
B) Hydrogen bond interactions through water molecules with lead1