Table S7. Hydrogen bonding pattern with critical residues (for representative ZINC leads). Details of critical interactions during MD simulations at every 0.5ns.

ZINC Leads	0.5ns	1.0ns	1.5ns	2.0ns	2.5ns	3.0ns	3.5ns	4.0ns	4.5ns	5.0ns
ZINC04286771	Ser302 His110	--	His110	--	His110	His110	His110	His110	His110	His110
ZINC49016166	His110 Cys298	His110	--	His110 Cys298	His110	His110	His110	His110	His110	His110