Table S3. Hydrogen bonding pattern with critical residues (for best PDMs). Details of critical interactions during MD simulations at every 0.5ns.

Best PDMs	**0.5ns**	**1.0ns**	**1.5ns**	**2.0ns**	**2.5ns**	**3.0ns**	**3.5ns**	**4.0ns**	**4.5ns**	**5.0ns**
RASE0048	His110 Trp111	His110 Trp111	His110 Trp111	His110 Trp111	His110 Trp111	His110 Trp111	Cys298	His110 Trp111	His110 Trp111	His110 Trp111
RASE0049	Trp20	His110	--	--	His110 Trp20	His110 Trp111	His110	His110	His110 Trp111	His110 Trp111
RASE0143	His110	His110 Trp111	His110 Gln49	Trp20	--	--	--	--	--	Gln49