Table S1. Energetic contributions.

Simulation	System conformational entropy, kJ/molK	Binding enthalpy per ligand, kJ/mol	Binding free energy per ligand, kJ/mol
holoArgRC	64.8 ± 0.4	-733 ± 198	-241 ± 38
apoArgRC	65.6 ± 0.3		
holoArgRC – 5a L-arg	66.7 ± 0.7	-873	-415
holoArgRC – 5b L-arg	65.6 ± 0.3	-696	-313
holoArgRC – 5c L-arg	66.3 ± 0.2	-816	-377
apoArgRC + 1a L-arg	66.2 ± 0.3	-671	-318
apoArgRC + 1b L-arg	65.6 ± 0.3	-818	-379
apoArgRC + 2a L-arg	66.1 ± 0.4	not determined	-237
apoArgRC + 2b L-arg	66.7 ± 0.3	not determined	-264
apoArgRC + 2c L-arg	65.4 ± 0.2	not determined	-295