Supplementary Information

Heterogeneous path ensembles for conformational transitions in semi–atomistic models of adenylate kinase

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We plot distances from several experimental crystal structures in Figures 7 and 10 of the main text. These structures are tabulated in Table S1. Several of the structures are for adk variants with different sequences, and, hence, require other residue pairs than those used in the main text to establish "equivalent" pairs to denote the BD–LID and LID–CORE distances. The residues for each equivalent pair were selected by a visual inspection of crystal structures, without considering our simulation data. Because the structures of different adk molecules are highly similar, there is minimal ambiguity in selecting the positional analogs of the beaded residues in Figures 8 and 9 of the main text. The selected residue pairs for the additional crsytal structures are shown in Table S1.

We emphasize that the choice of residue pairs was not influenced by proximity to paths.

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Table S1: PDB ID of structures used in Figures 7 and 10 of the main text and the corresponding residue pairs used for BD–LID and LID–CORE distances.

PDB ID	Chain	BD–LID (Å)	LID–CORE (Å)
1AK2	A	$d_{72,183} = 22.15$	$d_{31,152} = 9.01$
1DVR	A	$d_{60,172} = 21.30$	$d_{19,141} = 7.07$
1DVR	B	$d_{60,172} = 21.65$	$d_{19,141} = 7.17$
1E4Y	A	$d_{56,163} = 5.37$	$d_{15,132} = 6.65$
2AK3	A	$d_{61,166} = 11.07$	$d_{20,135} = 20.75$
2AK3	B	$d_{61,166} = 12.44$	$d_{20,135} = 21.25$
2RH5	A	$d_{56,157} = 23.62$	$d_{15,133} = 18.07$
2RH5	B	$d_{56,157} = 23.75$	$d_{15,133} = 15.01$
2ECK	A	$d_{56,163} = 5.15$	$d_{15,132} = 5.98$
1ANK	A	$d_{56,163} = 5.13$	$d_{15,132} = 6.22$
1ZIN	A	$d_{56,167} = 5.48$	$d_{15,136} = 8.91$
1ZIO	A	$d_{56,167} = 5.38$	$d_{15,136} = 9.26$
2EU8	A	$d_{56,167} = 5.22$	$d_{15,136} = 7.01$
2OO7	A	$d_{56,167} = 5.22$	$d_{15,136} = 7.02$
2ORI	A	$d_{56,167} = 5.10$	$d_{15,136} = 7.12$
2OSB	A	$d_{56,167} = 5.20$	$d_{15,136} = 6.89$
2RGX	A	$d_{56,167} = 5.17$	$d_{15,136} = 7.58$
1AKY	A	$d_{60,172} = 4.59$	$d_{19,141} = 6.92$
2AKY	A	$d_{60,172} = 4.97$	$d_{19,141} = 6.80$
1ZAK	A	$d_{61,165} = 7.09$	$d_{20,138} = 6.41$
2BBW	A	$d_{61,166} = 14.89$	$d_{20,135} = 12.43$
2BBW	B	$d_{61,166} = 14.47$	$d_{20,135} = 9.27$
2C9Y	A	$d_{71,182} = 22.58$	$d_{30,151} = 11.25$
2AR7	A	$d_{62,166} = 21.76$	$d_{20,135} = 19.85$
2AR7	B	$d_{62,166} = 18.03$	$d_{20,135} = 18.58$