Niu *et al.* Supplementary Data

Table S 1:

Method:	DynDom		ESCET		Consensus	
	Domain	Residues	Rigid body	Residues	Rigid group	Residues
	1	7-95 196-199 269	1	2-100 193-201 269-276	1	2-102 193-201 269-276
	4	96-100 126-150 168-172 185-195 200-230 257-268 270-277	3	101-102 130-155 167-173 202-213 221-229 258-259	2	129-155 167-173 202-213 221-229 258-259
	5	173-184	5[†]	174-187	3	174-187
	2	101-125 156-163 231-256 278-287 328-352	2	103-111 117-129 156-166 216-220 230-257 260-268 277-290 332-357	4	103-128 156-166 216-220 230-257 260-268 277-290 330-357
	3	288-327[‡]	4	115-116 293-309[‡] 322-331[‡]	5	293-310[‡], 320-329[‡]
Critical parameters:	Window: Domain:	11 residues 11 residues	Lolim: Minfraglen:	1.25 Å 2%		

Table S 1: Identification of the rigid groups in Arginine Kinase. The substrate-free (PDBid 3M10) and transition state analog complex (PDBid 1M15) structures were compared using DynDom [42]

and ESCET [41]. In spite of using quite different algorithms, residue assignments were 79% identical. A consensus was derived by inspection of the structures, either compromising or choosing from the two designations in the way that would best consolidate the residues in 3D space. [†] Rigid body 5 was identified by ESCET and used in our analysis even though it was rejected ESCET as failing to meet the minimum size of 20 residues. [‡] Residues 311-319 are resolved only in the transition state structure. Differences in this region are due only to the different ways that the programs handle residues missing from one of the structures.

Figure S 1:

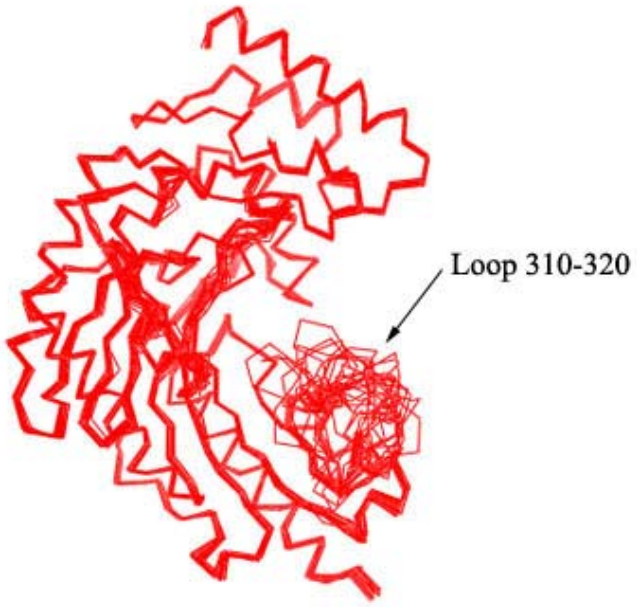

Figure S 1: Ensemble of 25 structures of apo AK in solution generated by XPLOR-NIH based on substrate-free and TSA crystal structures, NMR RDCs and chemical shifts as restraints. The refined solution structure is very similar to the substrate-free crystal structure. The backbone Cα RMSD of the average structure of the ensemble is only 0.9 Å to the substrate-free crystal structure (after removal of the disordered loop 310-320, which is invisible in the substrate-free crystal structure).