

Supplementary Material

Supplementary Table 1: Kinase motifs with alternative conformations. For each of the three kinases there are four motifs with differing conformations among the experimentally determined ensemble members. Three of the motifs are common to all three kinases and are related to their enzymatic activity (see text).

Kinase	Motif	Residue range (target numbering)	Experimental ensemble members difference ¹ , Å	Smallest CASP model difference to NMR/X-ray ² , Å	# of groups within 20% of the NMR best ³
T1195	β sheet	4-46, 74-85	4.9	2.9 / 1.1	15
	αC helix	47-64	7.4	2.3 / 1.2	1
	Activation loop	150-169	Mainly disordered in X-ray	3.0 / na	0
	Additional motif	87-103	2.3	1.6 / 0.7	3
T1196	β sheet	4-41, 88-108	4.3	1.3 / 1.4	3
	αC helix	57-80	2.7	0.9/ 0.8	3
	Activation loop	171-184	Disordered in X-ray	4.2 / na	16
	Additional motif	314-332	4.9	3.1 / 0.9	21
T1197	β sheet	19-38, 84-92	3.4 / 1.8	0.8 / 2.7 / 0.9	0
	αC helix	53-69	3.5 / 1.6	1.2 / 3.2 / 0.8	21
	Activation loop	162-180	10.8 / 4.1	3.3 / 1.7 / 1.9	14
	Additional motif	222-235	3.3 / 1.1	0.8 / 3.1 / 0.9	3

¹ - average Cα distance for residues in a motif between two experimental ensemble conformations. For T1197, with three members in the ensemble, the distances between the NMR structure and the two PDB-derived models are given;

² - average Cα distance between the closest computed model in the submission and the experimental NMR and PDB-derived structures (each submission consists of five models). For T1197, distances to all three experimental structures are given;

³ - number of additional groups with CASP models within 20% of the closest distance to experiment.