Supporting Information for World Wide Web Edition

Table 1. Comparison of structures calculated with and without calcium and H-bond constraints.

Model	Coordinate Precision	
Omit Ca	RMSD to Mean (Backbone Atoms)[a]	0.59 Å
	RMSD to Mean (Heavy Atoms)[a]	1.13 Å
	RMSD to final reported structure (Backbone Atoms)[b]	0.55 Å
	RMSD to final reported structure (Heavy Atoms)[b]	1.20 Å
Omit H-bonds	RMSD to Mean (Backbone Atoms)[a]	0.61 Å
	RMSD to Mean (Heavy Atoms)[a]	1.12 Å
	RMSD to final reported structure (Backbone Atoms)[b]	0.49 Å
	RMSD to final reported structure (Heavy Atoms)[b]	1.21 Å
Omit Both	RMSD to Mean (Backbone Atoms)[a]	0.70 Å
	RMSD to Mean (Heavy Atoms)[a]	1.20 Å
	RMSD to final reported structure (Backbone Atoms)[b]	0.84 Å
	RMSD to final reported structure (Heavy Atoms)[b]	1.44 Å
Include Both	RMSD to Mean (Backbone Atoms)[a]	0.55 Å
	RMSD to Mean (Heavy Atoms)[a]	1.01 Å

[a] residues 215-249.
[b] residues 215-247.

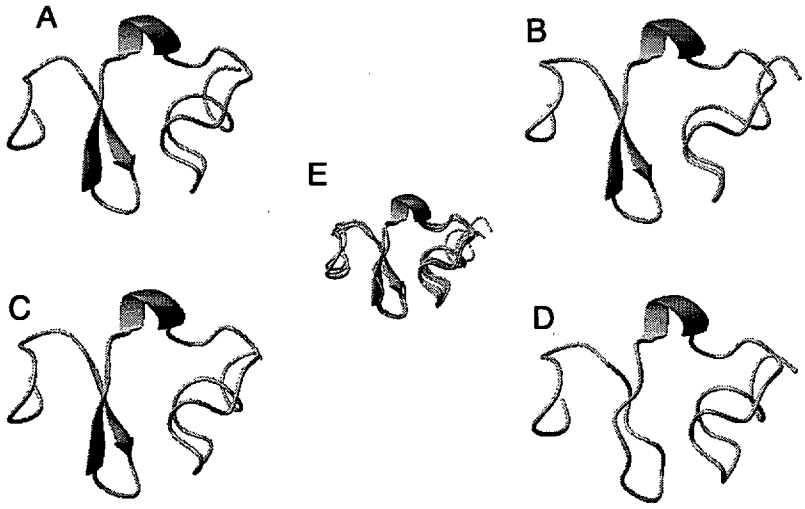

Figure 1. Ribbon representations of minimized mean structures of LR6* calculated when different sets of distance constraints are omitted from the calculations. A. Model calculated as reported in the text. B. Model calculated omitting explicit H-bond constraints. C. Model calculated without a calcium ion or constraints to specify the octahedral calcium binding-site geometry. D. Model calculated when H-bond and calcium coordination constraints are both omitted from the calculations. E. Best-fit superposition of models A-D.

Fig 1, supporting information