

Table 1. NMR and refinement statistics for the homodimeric A4 domain of factor XI

Intramonomer restraints	
Total NOE distance constraints	1,339
Intraresidue	403
Sequential ($ i-j = 1$)	407
Medium-range ($ i-j < 4$)	121
Long-range ($ i-j > 5$)	316
Hydrogen bonds	61
Total dihedral angle restraints (Ψ & Φ)	112
Total RDC	70
Intermonomer NOE restraints	48
Order parameter from RDC analysis (using PALES)	
Da=-7.2095; R=0.245	
$S_{xx}=2.1145e^{-04}$ $S_{yy}=4.5655e^{-04}$ $S_{zz}=-6.6800e^{-04}$	
Structure Statistics of 14 converging structures	
Deviations from idealized geometry	
Bond lengths, Å	0.0032±0.0003
Bond angles, °	0.70±0.12
Impropers, °	0.93±0.1
Average pairwise rmsd, Å	
Heavy atoms (well defined region)	1.95 (1.045)
Backbone (well defined region)	1.43 (0.8471)
Ramachandran plot	
Most favored region, %	57.7
Additionally allowed region, %	32.1
Generously allowed region, %	6.4
Disallowed region, %	3.8
