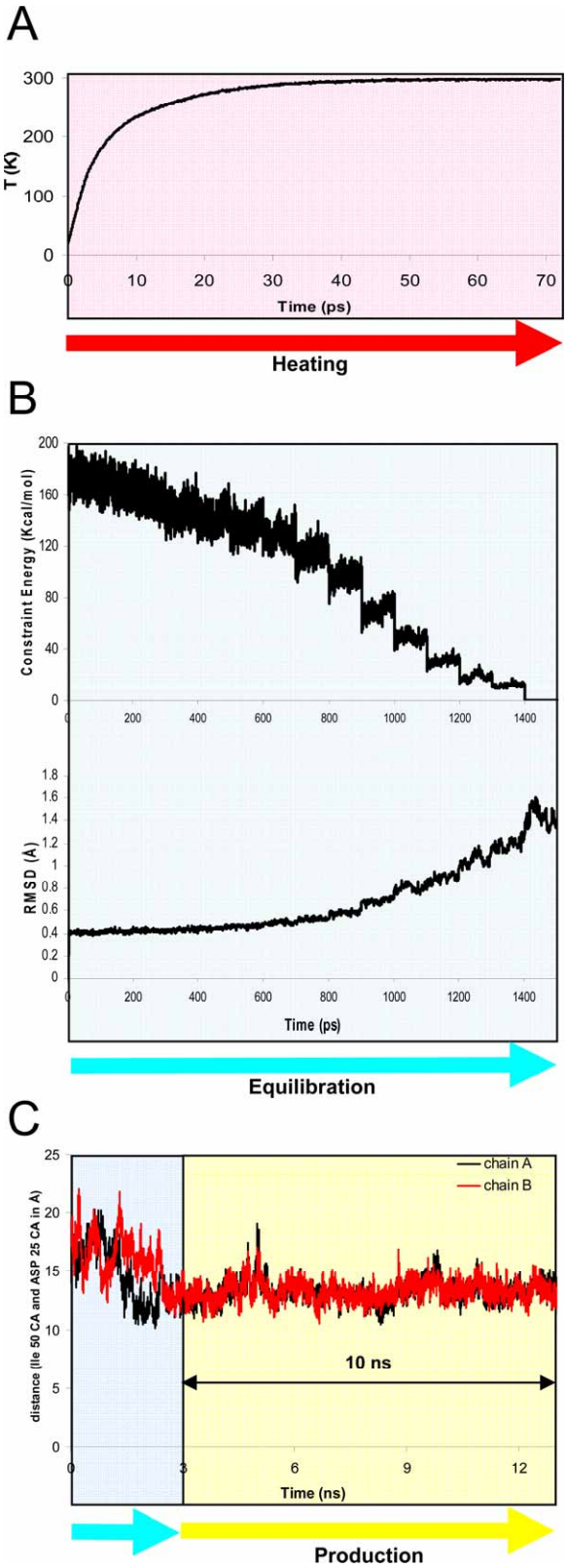
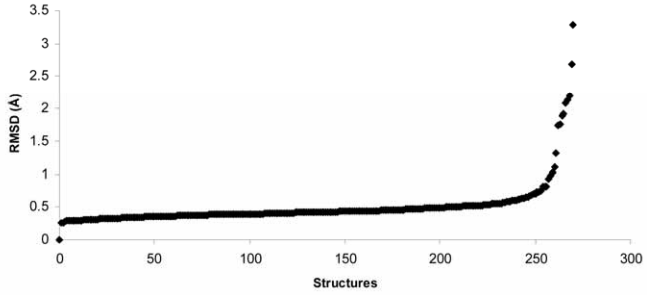


Fig. S1. Summary of equilibration procedure

A

1A30, 1A8G, 1A8K, 1A94, 1A9M, 1AAQ, 1AID, 1AJV, 1AJX, 1AXA, 1B6J,
1B6K, 1B6L, 1B6M, 1B6P, 1BDL, 1BDQ, 1BDR, 1BV7, 1BV9, 1BWA, 1BWB,
1C6X, 1C6Y, 1C6Z, 1CPI, 1D4H, 1D4I, 1D4J, 1D4K, 1D4L, 1D4S, 1D4Y,
1DAZ, 1DIF, 1DMP, 1DW6, 1EBK, 1EBW, 1EBY, 1EBZ, 1EC0, 1EC1, 1EC2,
1EC3, 1F7A, 1FB7, 1FEJ, 1FF0, 1FFF, 1FFI, 1FG6, 1FG8, 1FGC, 1FQX,
1G2K, 1G35, 1G6L, 1GNM, 1GNN, 1GNO, 1HBV, 1HEF, 1HEG, 1HHP, 1HIH,
1HIV, 1HOS, 1HPO, 1HPS, 1HPV, 1HPX, 1HTE, 1HTF, 1HTG, 1HVC, 1HVH,
1HVI, 1HVJ, 1HVK, 1HVL, 1HVR, 1HVS, 1HWR, 1HXB, 1HXW, 1IIQ, 1IZH,
1IZI, 1JLD, 1K1T, 1K1U, 1K2B, 1K2C, 1KJ4, 1KJ7, 1KJF, 1KJG, 1KJH,
1KZK, 1LV1, 1LZQ, 1M0B, 1MER, 1MES, 1MET, 1MEU, 1MRW, 1MRX, 1MSM,
1MSN, 1MT7, 1MT8, 1MT9, 1MTB, 1MTR, 1N49, 1NH0, 1NPA, 1NPV, 1NPW,
1ODW, 1ODX, 1ODY, 1OHR, 1QBR, 1QBS, 1QBT, 1QBU, 1RL8, 1RPI, 1RQ9,
1RV7, 1SBG, 1SDT, 1SDU, 1SDV, 1SGU, 1SH9, 1SP5, 1T3R, 1T7I, 1T7J,
1T7K, 1TCX, 1TW7, 1U8G, 1UPJ, 1VIJ, 1VIK, 1W5V, 1W5W, 1W5X, 1W5Y,
1WBK, 1WBM, 1XL2, 1XL5, 1YT9, 1Z1H, 1Z1R, 1Z8C, 1ZBG, 1ZJ7, 1ZLF,
1ZP8, 1ZPA, 1ZPK, 1ZSF, 1ZSR, 1ZTZ, 2A1E, 2A4F, 2AID, 2AOC, 2AOD,
2AOE, 2AOF, 2AOG, 2AOH, 2AOI, 2AOJ, 2AVM, 2AVO, 2AVQ, 2AVS, 2AVV,
2AZ8, 2AZ9, 2AZC, 2BB9, 2BPV, 2BPW, 2BPX, 2BPY, 2BPZ, 2BQV, 2CEJ,
2CEM, 2CEN, 2F3K, 2F80, 2F81, 2F8G, 2FDD, 2FDE, 2FGU, 2FGV, 2FLE,
2FNS, 2FNT, 2FXD, 2FXE, 2HB4, 2HC0, 2HS1, 2HS2, 2IDW, 2IEN, 2IEO,
2NMW, 2NMY, 2NMZ, 2NNK, 2NNP, 2NPH, 2NXD, 2NXL, 2NXM, 2P3A, 2P3B,
2P3C, 2P3D, 2PC0, 2PQZ, 2PSU, 2PSV, 2PWC, 2PWR, 2PYM, 2PYN, 2Q63,
2Q64, 2QAK, 2QNN, 2QNP, 2QNQ, 2UPJ, 2UXZ, 2UY0, 2Z54, 3AID, 3B7V,
3B80, 3BVA, 3BVB, 3BXR, 3BXS, 3CYW, 3CYX, 3D1X, 3D1Y, 3D1Z, 3D20,
3D3T, 3TLH, 4HVP, 4PHV, 5HVP ,7UPJ.

B



C

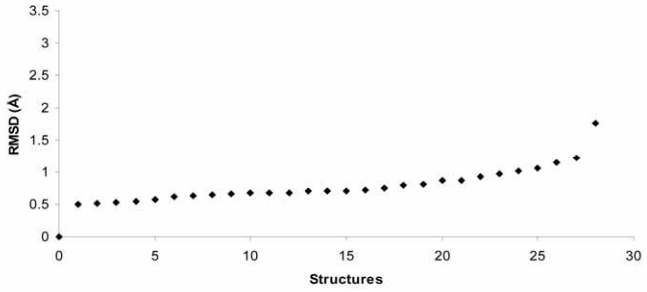


Fig. S2. A list of the PDB identifiers (A) and the RMSD for each structure after superposition (B), as well as for the NMR data set (C)

```
for each minimum (of Ns)                                    [note 1]

    reorient structure to reference structure               [note 2]

    calculate NM


    for each NM (of Nmodes)

       generate trajectory at a given temperature           [note 3]
       around the reference structure

    store trajectory

    end

end

concatenate the Ns x Nmodes trajectories

calculate quasimodes of concatenated trajectory

-------------------------------
note 1: Energy minimize the structures sampled from MD
note 2: Reorient each structure to a reference structure (e.g.,
1st structure)
note 3: Each mode's harmonic trajectory consists of a small number
of points (here 9). Modes must be generated for a single
temperature, although the mode directions will be independent of
the precise value chosen.
```

Fig. S3. A pseudocode describing the routine used to calculate the CM from the QHM analysis of modes trajectory