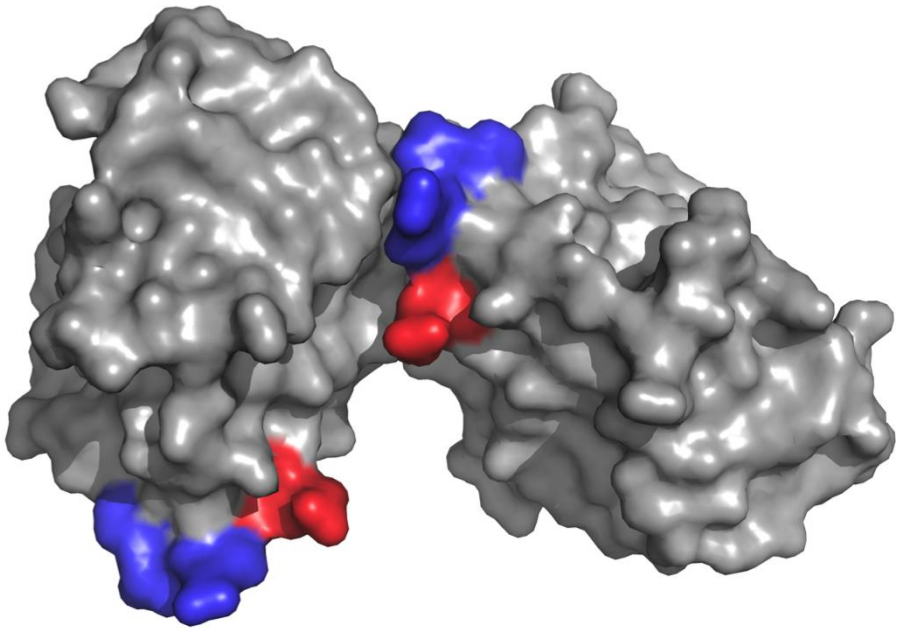
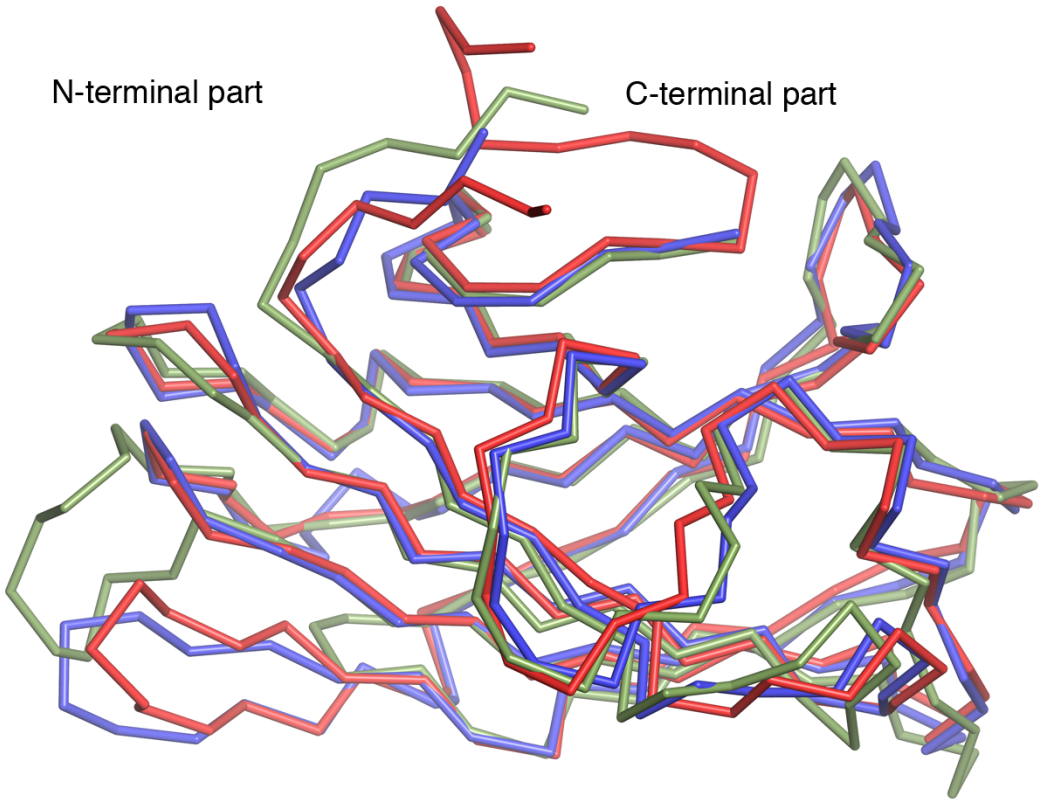
Supplementary Material

As discussed in the paper, the C and N termini in the current structure are near to each other in space (Supplementary Fig 1) and form a stem-like structure. We are able to rule out the influence of crystal packing contacts on the termini conformation. At the C terminus, the main chain changes direction after Pro200 and folds back onto β-strand 9 due to its interaction with residue Thr130 and loop 5/6 and not due to interactions at the packing interface. The direction change at the N terminus takes place at residue Asn46. The Cα position of this residue is 8.4Å from the Cα of Asn161 (from the symmetry related molecule) and could feasibly be affected by its proximity; superposition with related CBM's (PDB codes 1G43, 2XBT; (Shimon *et al.*, 2000, Yaniv *et al.*, 2011)) however, shows that the trace of the main chain is consistent with these other structures (Supplementary Fig 2).



Supplementary Figure S1. Contact between two symmetry related molecules of CBM3a-L. N-terminus is colored in blue color, C-terminus in red.



Supplementary Figure S2. Superposition of the CBM3a-L structure with 2XBT and 1G43 in red, green and blue respectively. The three structures pack in different space groups ($P4_132$, $I4_122$, $P6_522$) and make different crystal-packing interactions. The presence (in CBM3a-l and 2XBT) or absence (in 1G43) of crystal-packing contacts in the N-termini region does not appear to affect the fold of the chain; all the N-termini of all 3 of these CBM's are folded back towards the protein globule.

References

Shimon, L. J., Pages, S., Belaich, A., Belaich, J. P., Bayer, E. A., Lamed, R., Shoham, Y. & Frolow, F. (2000). *Acta Cryst.* D**56**, 1560-1568.

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