Supplementary material

Table S1

The lists of residues reported in the table have been calculated by running a simulation of GAA in the presence of 10 NAC molecules starting from random positions in the simulation box. The NAC-density maps on the protein surface were calculated using the program gridcount (*N. Michaud-Agrawal, E. J. Denning, T. B. Woolf, O. Beckstein. MDAnalysis: A Toolkit for the Analysis of Molecular Dynamics Simulations J. Comp. Chem. (2011). doi:10.1002/jcc.21787).* The residues in contact with NAC have been defined using surfaces of NAC with an isovalue of 1.3mol/l. The bold line indicates the site identified also in the flexibility analysis as a possible hotspot for stability regulation.

Contact Site	***Residues***
1	ASP94, ARG37, GLN33, GLU468, LYS93, PRO92
2	ARG120, GLN494
3	ARG395, THR425, PRO424, ALA428, ARG394
4	ARG324, TRY616, SER716, SER617, SER619, HIS326, PRO718, PRO719
5	SER74, ARG134, TYR79, PRO136, SER137, SER141, GLU143, GLN156, ASP158
6	ASN583, GLY582, THR584, PHE580, LEU581
7	GLN52, GLY50, TRP57
8	SER311, SER310, GLN317, LEU609, LEU608, ALA313, ILE314
9	ASN813, ARG812
10	THR737, LEU738, GLN734, SER731, ILE729, GLU732, THR702, LYS864, THR863, LYS780, GLU783, CYS883
11	GLN46, LYS45, ARG5
12	GLN55, PRO56, ARG20, VAL15, ASP14, TYR41, PRO16, PRO17
13	**LEU799, GLU800, ARG801, GLY802, ALA803, TYR804**
14	SER619, ARG37, GLN33, GLU468, LYS93, PRO92