

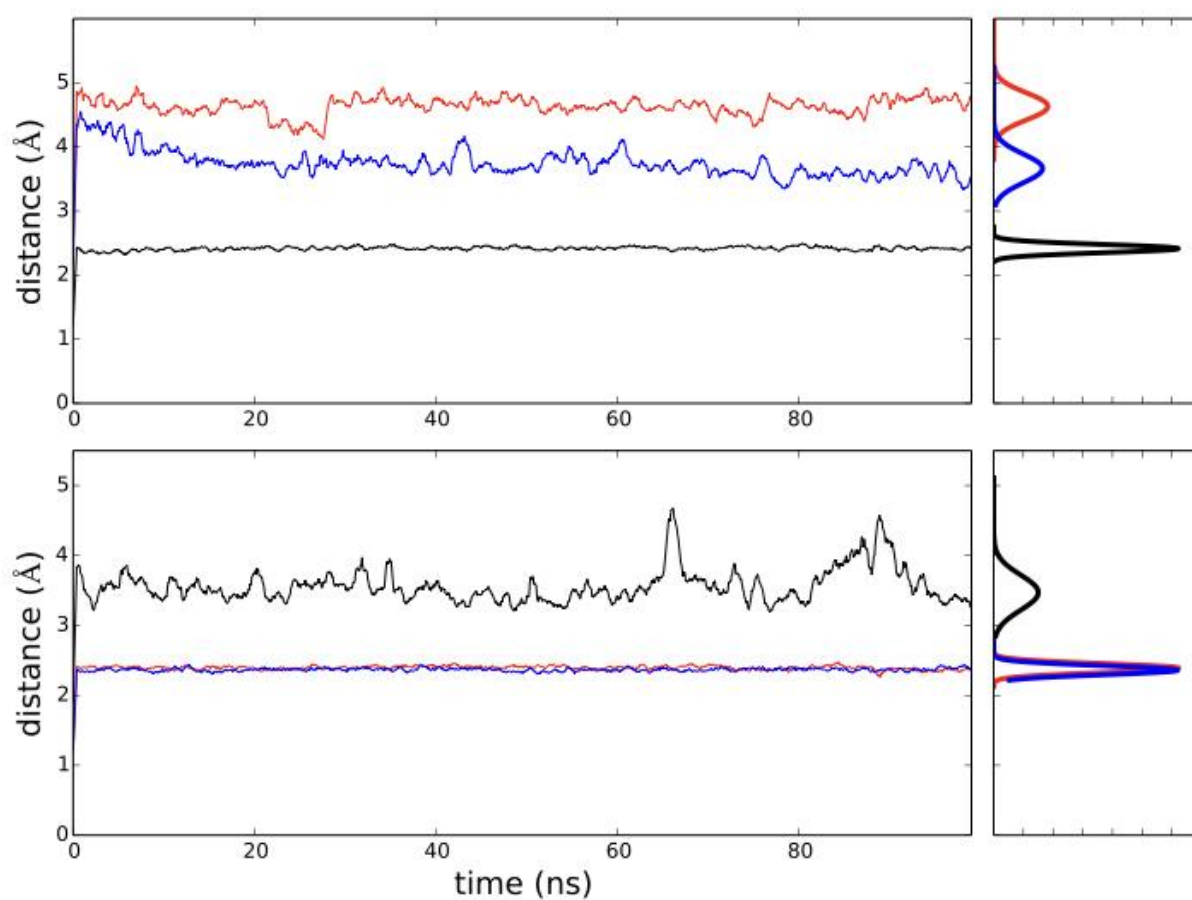
SUPPORTING INFORMATION

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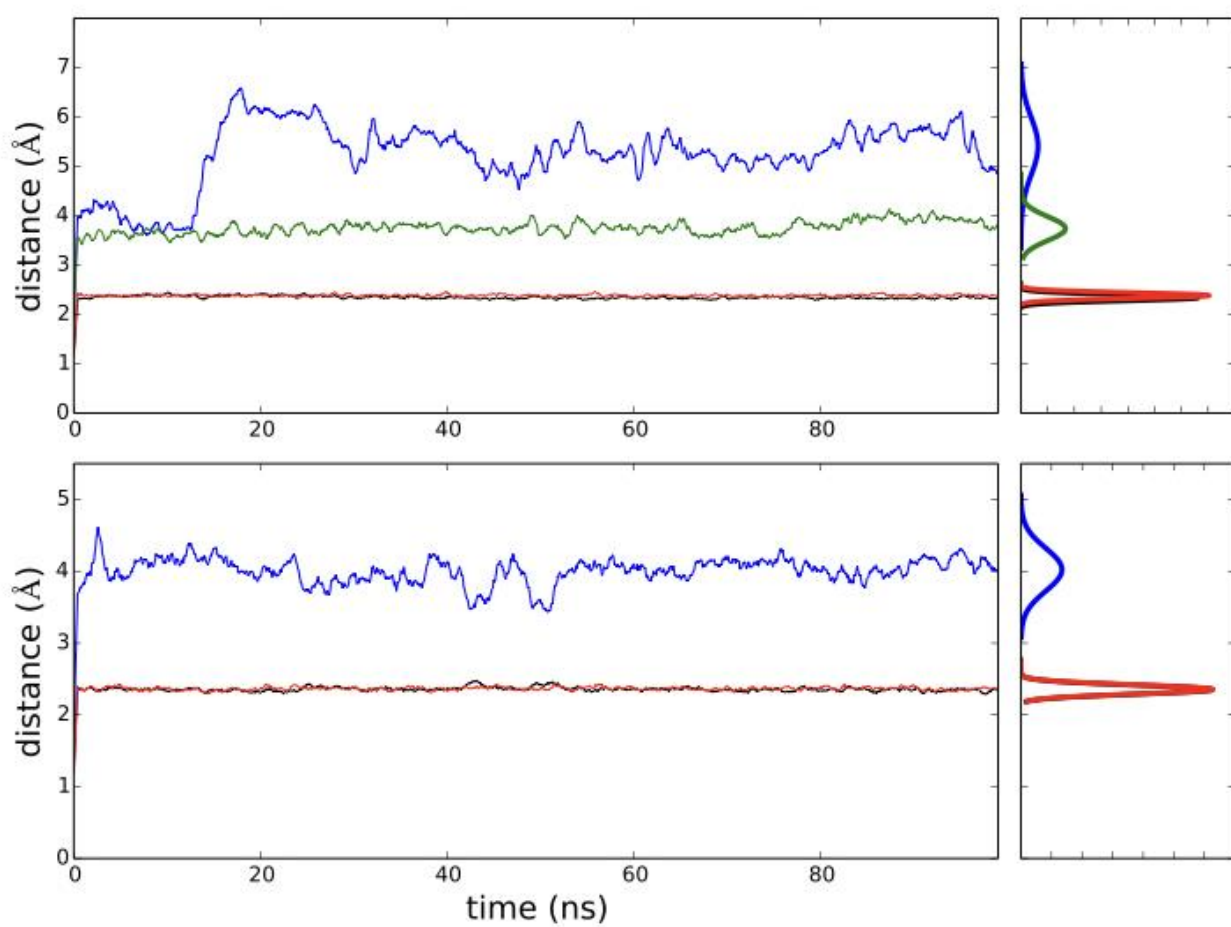
**Modelling of Ca<sup>2+</sup>-promoted structural effects in wild type and post-translationally modified Connexin26**

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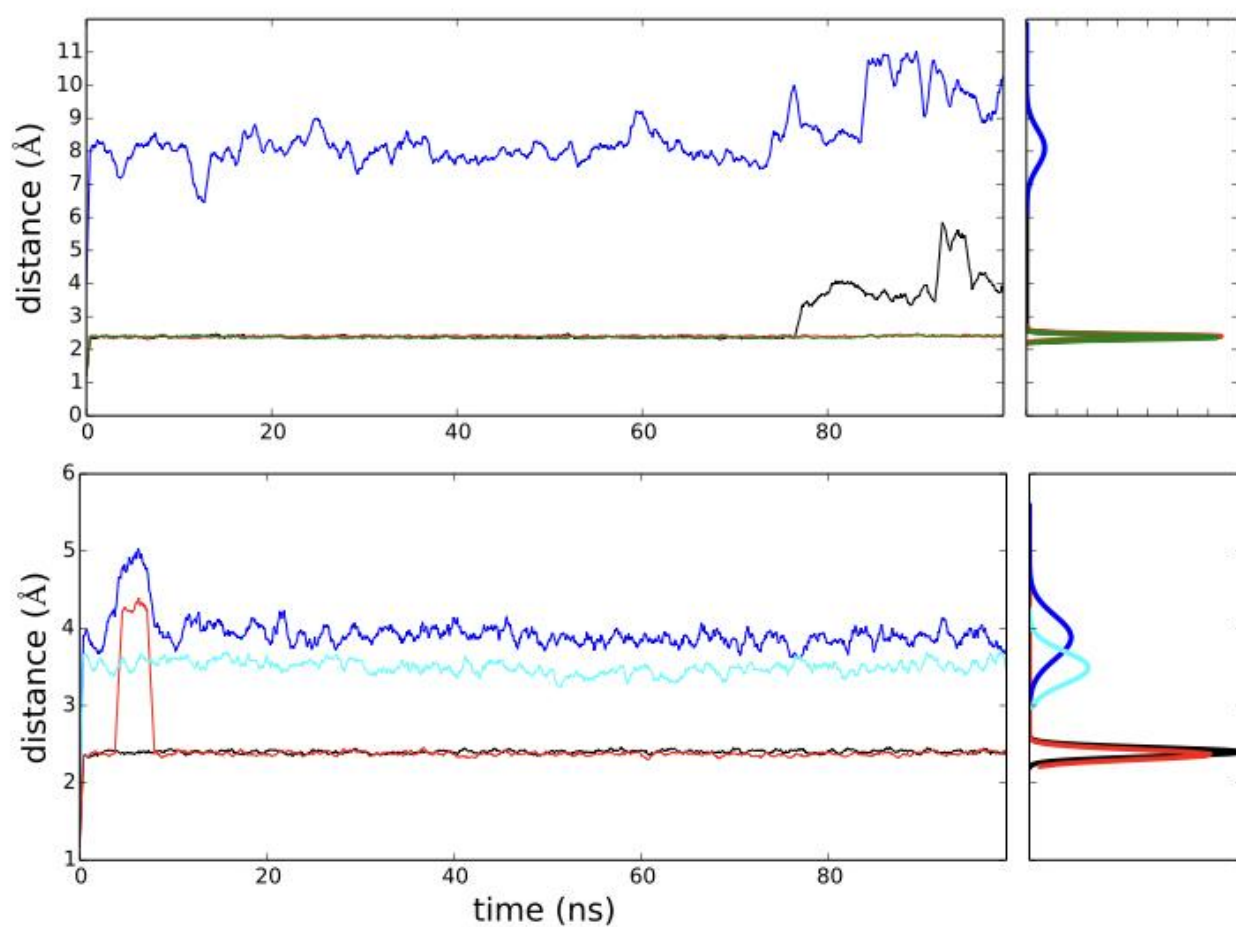
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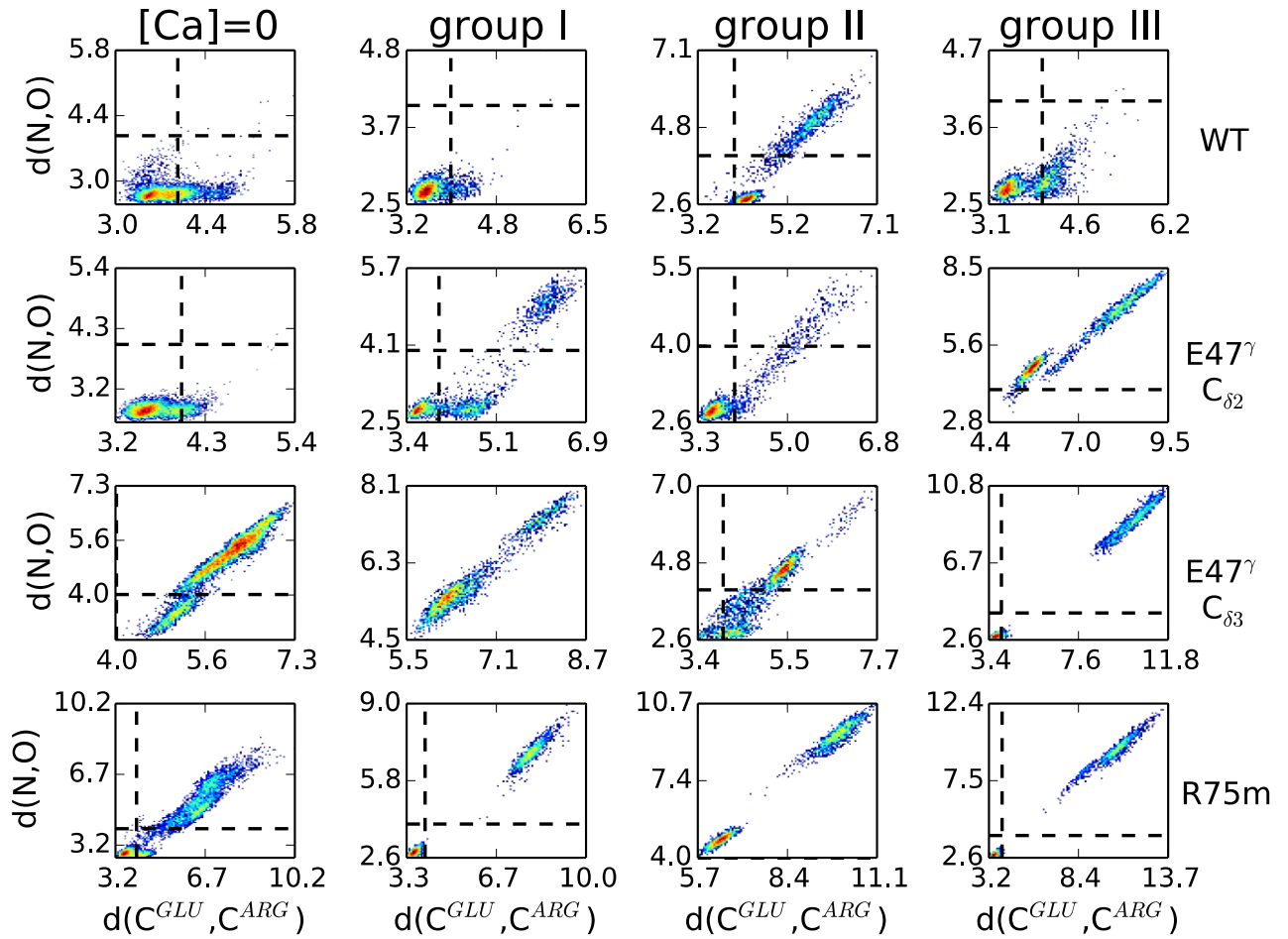
**Figure S1 :** Time evolution of minimum distances shown in Figure 7 for Cx26WT. Minimum distances between both calcium ions and their nearest residues are shown : E42, E47, R75 are shown in black, red, blue, respectively.



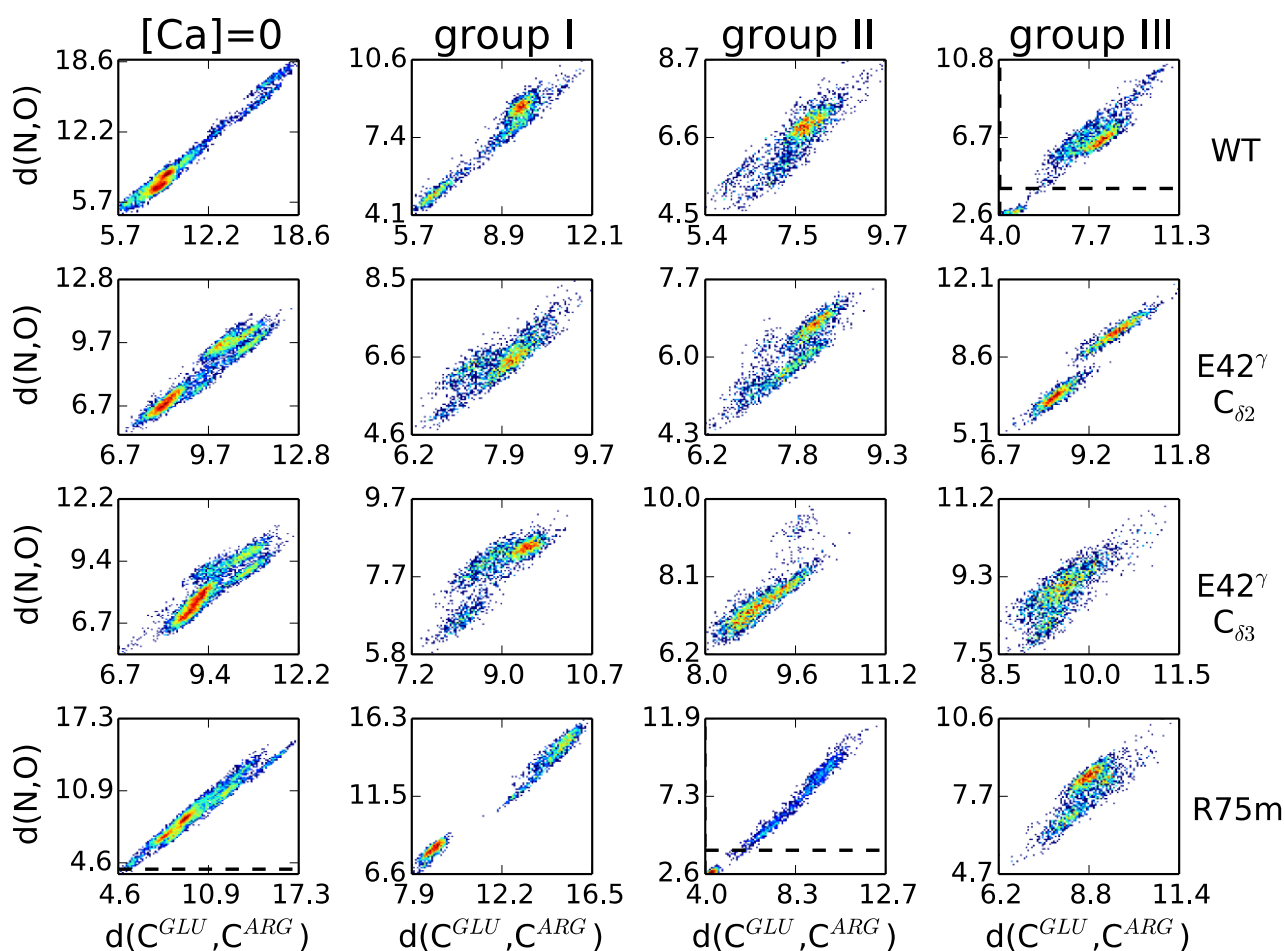
**Figure S2** : Time evolution of minimum distances shown in Figure 7 for Cx26E42-47γ. Minimum distances between both calcium ions and their nearest residues are shown : γE42, γE47, R75, D46A are shown in black, red, blue, green, respectively.



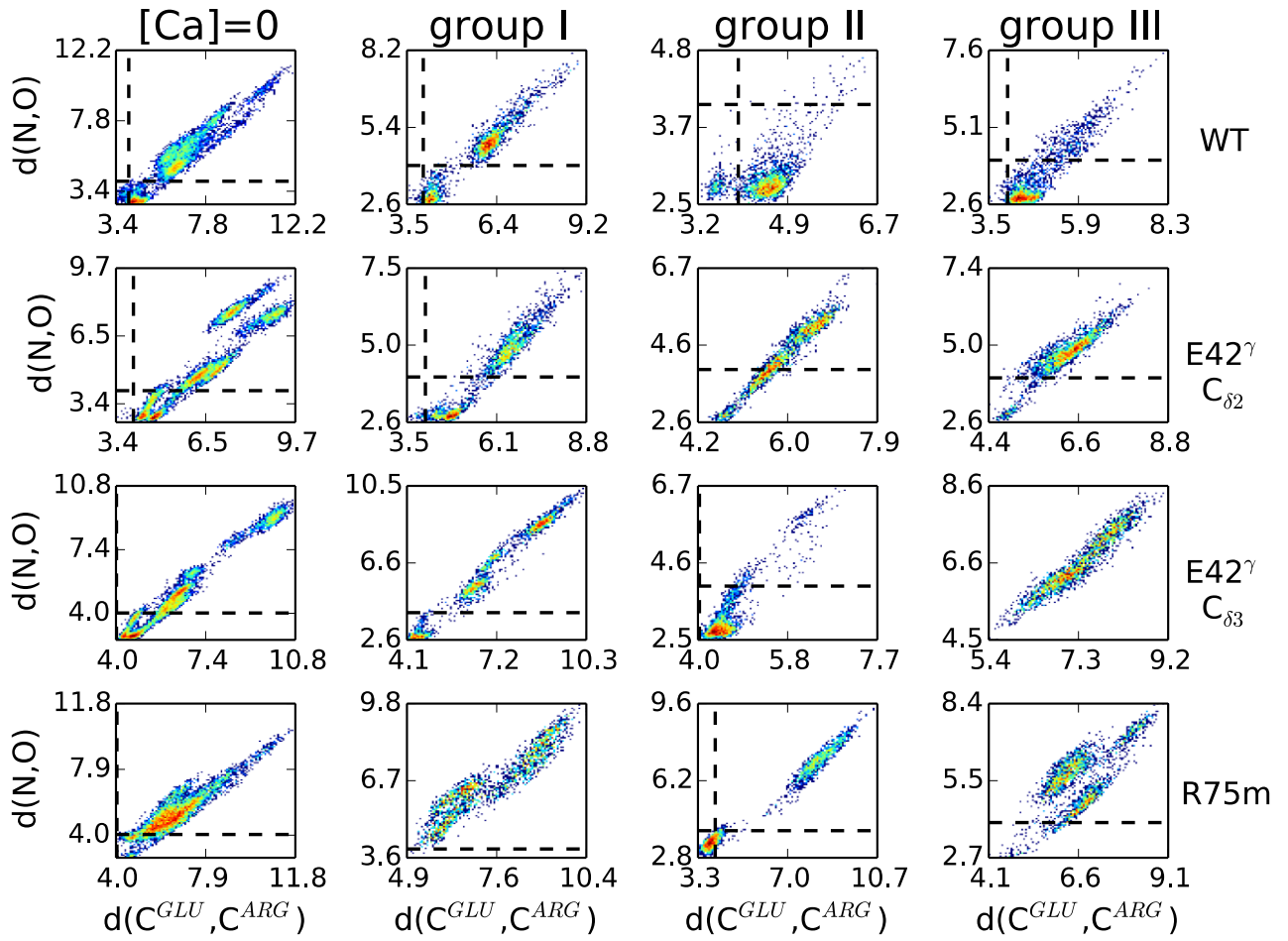
**Figure S3:** Time evolution of minimum distances shown in Figure 7 for Cx26R75m. Minimum distances between both calcium ions and their nearest residues are shown : E42, E47, R75, D46B are shown in black, red, blue and cyan, respectively.



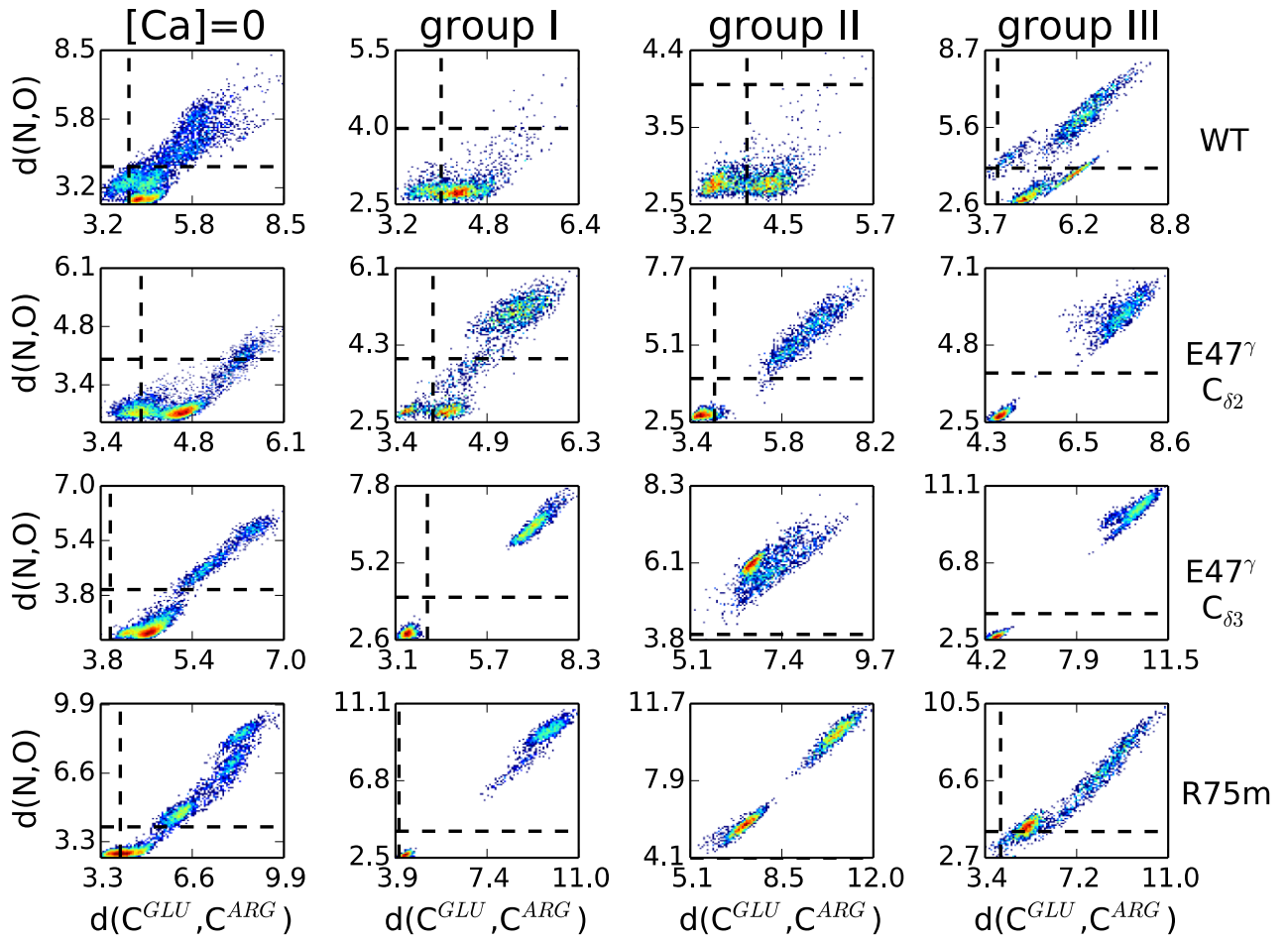
**Figure S4:** Ion-pair interaction between E47A and R75A in Cx26WT (first line), Cx26E42-47 $\gamma$  (second and third line) and Cx26R75m (forth line). Dashed lines define the boundaries of the different types of interactions ( $d(N,O) = 4.0$  and  $d(C^{GLU}, C^{ARG}) = 4.0$ ). Results from Cx26 in absence of calcium are shown in the left column. Results from Cx26 in presence of calcium ions are cast in three different groups: domains that do not directly interact with calcium ions in Ca<sup>2+</sup> bound protein (group I); domains whose E42 interacts with calcium ions (group II); protomes whose E47 and R75 are involved in the coordination of with a Ca<sup>2+</sup> ion (group III).



**Figure S5:** Ion-pair interaction between E42A and R184A in Cx26WT (first line), Cx26E42- 47 $\gamma$  (second and third line) and Cx26R75m (forth line). See Figure S4 for legend.



**Figure S6:** Ion-pair interaction between E42A and R75B in Cx26WT (first line), Cx26E42- 47 $\gamma$  (second and third line) and Cx26R75m (forth line). See Figure S4 for legend.



**Figure S7:** Ion-pair interaction between E47B and R184A in Cx26WT (first line), Cx26E42- 47 $\gamma$  (second and third line) and Cx26R75m (forth line). See Figure S4 for legend.