Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
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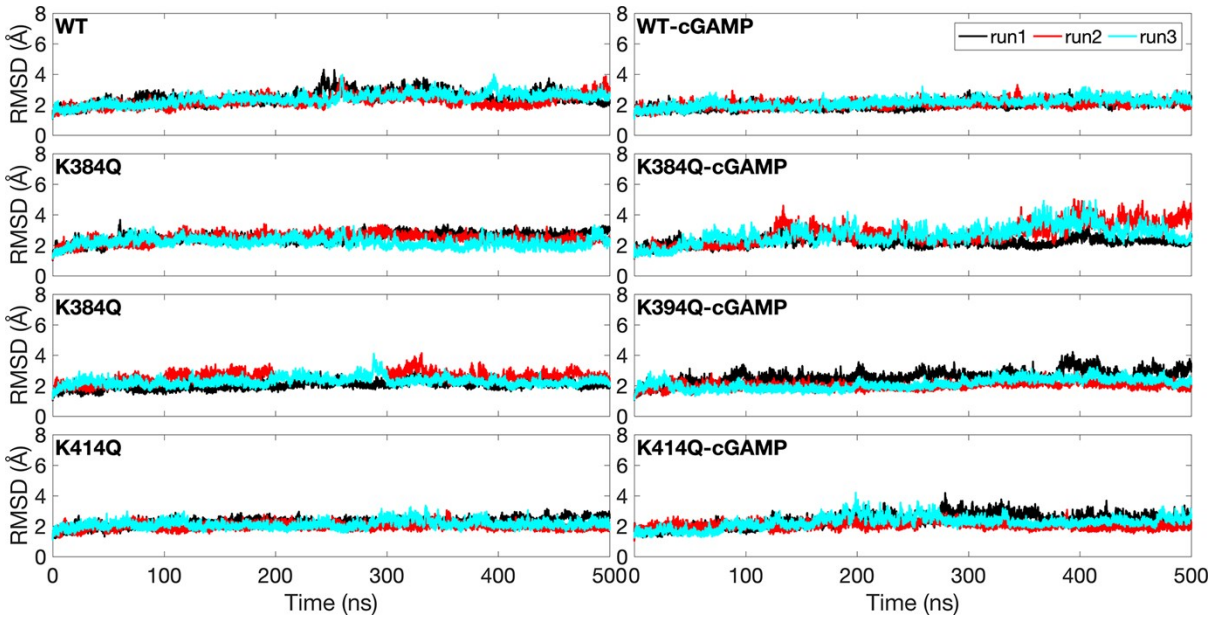

Fig. S1 The root-mean-square deviations (RMSDs) of Cα atoms of cGAS dimer in each simulation as a function of simulation time.

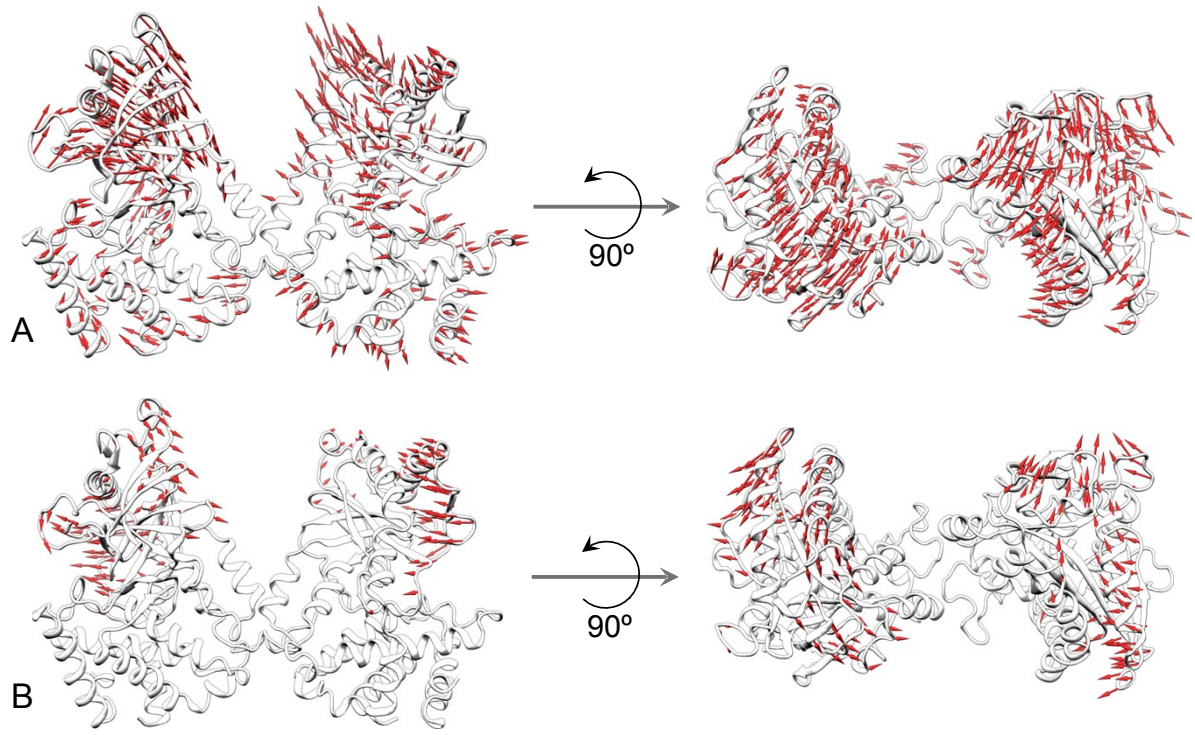

Fig. S2 The essential dynamics of the cGAS dimer derived from the first two principal components: (A) PC1; (B) PC2. The essential dynamics of each residue is shown as arrow with the cGAS dimer represented as cartoon. Related to Fig. 4.

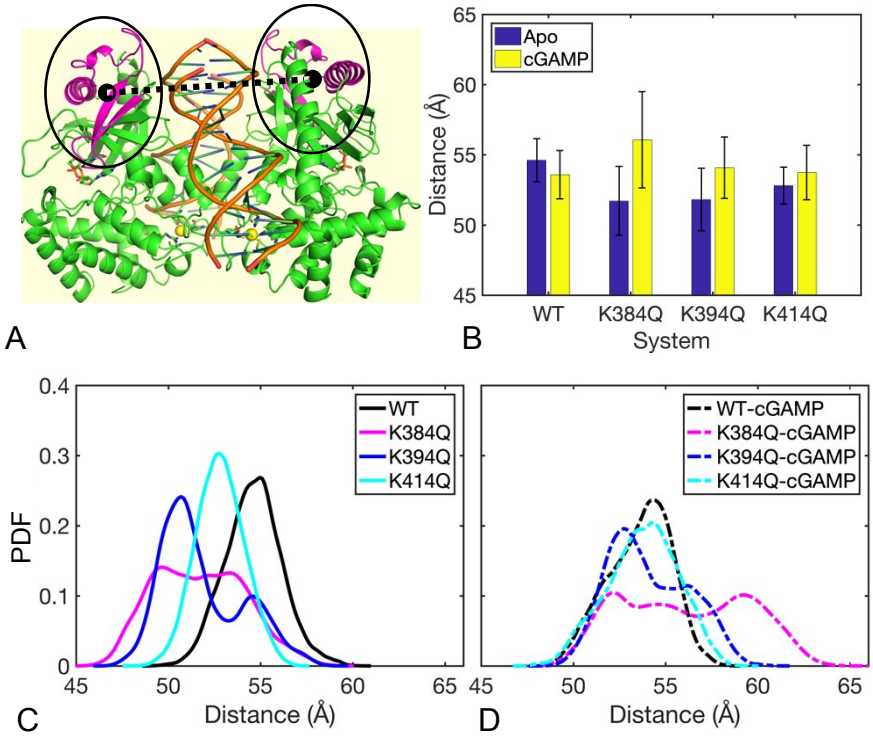

Fig. S3 The inward/outward motion of lobe 1 suggested by the distance between the center of Cα atoms in the β2-α2 region from lobe 1 during the last 100-ns simulations: (A) the model of cGAS-dsDNA dimer with the β2-α2 regions highlighted; (B) the average distance for each system; (C-D) the probability distribution function (PDF) of the distance between the two β2-α2 regions in the absence and presence of cGAMP. Related to Fig. 6.

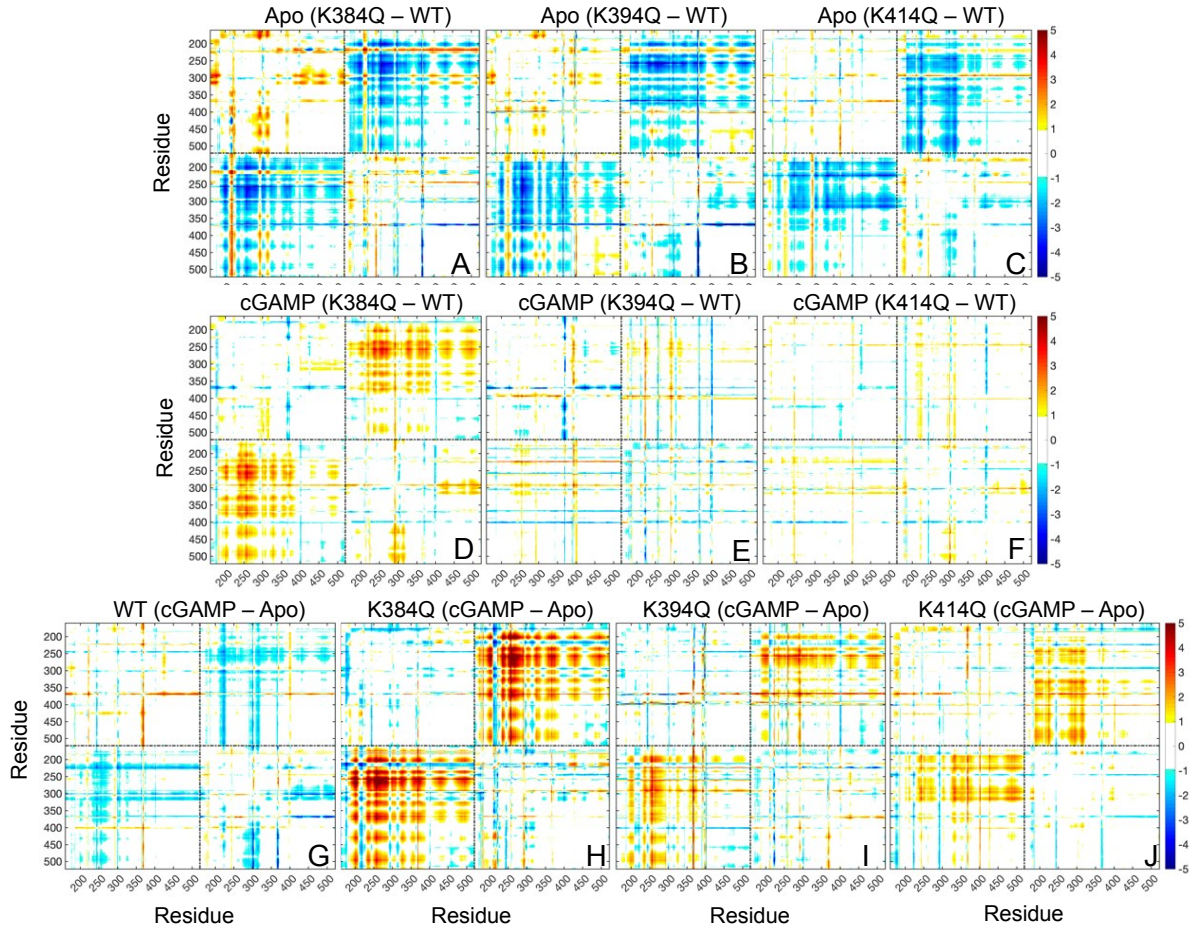

Fig. S4 The effects of mutation and ligand binding on Cα-Cα distance matrix of the cGAS dimer: effects of mutations on the 2:2 cGAS-dsDNA dimer in the absence (A-C) and presence (D-F) of cGAMP; (G-J) effects of cGAMP binding on the WT and mutated 2:2 cGAS-dsDNA dimer.

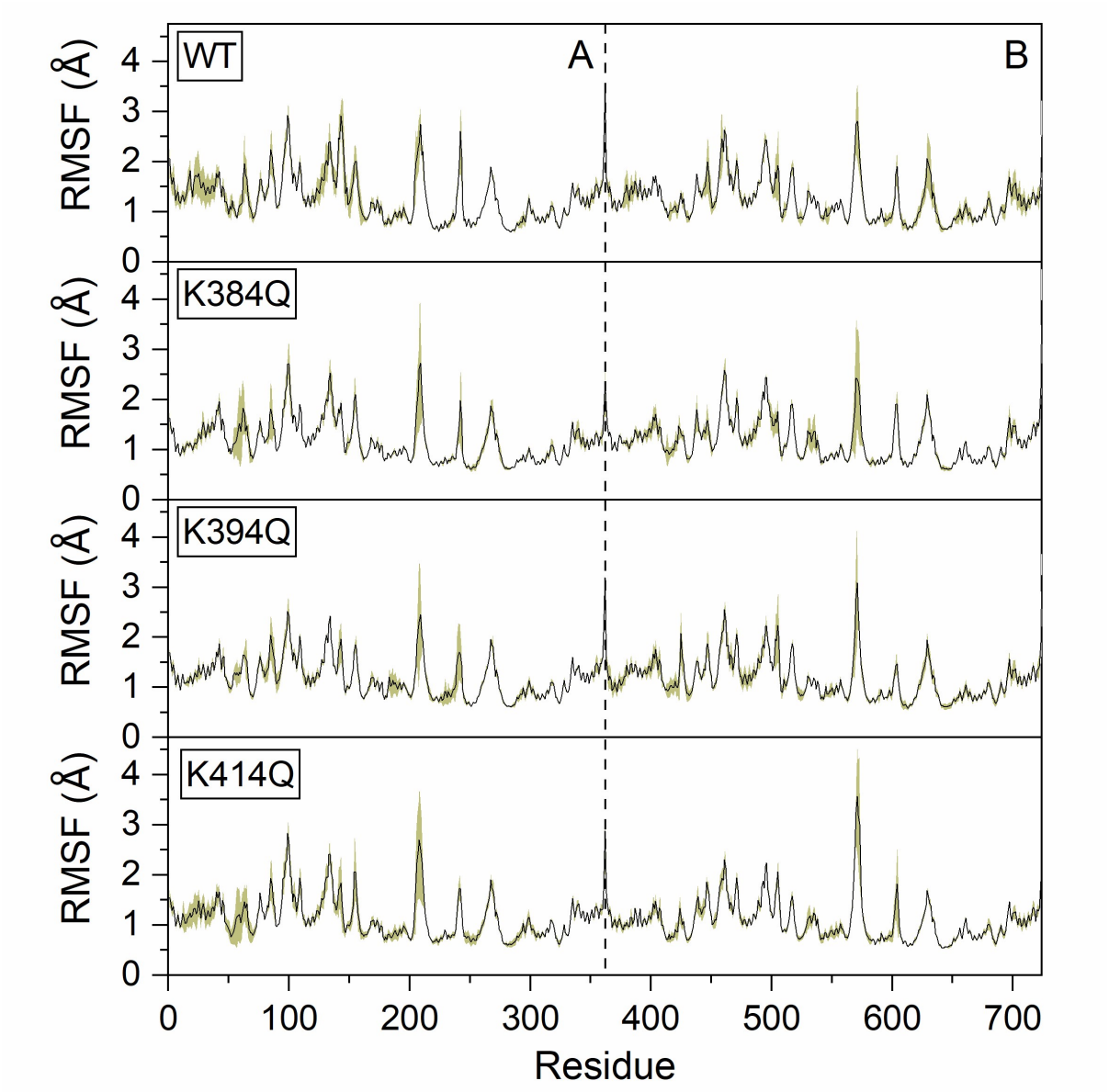

Fig. S5 The Cα root-mean-square fluctuations (RMSFs) of the apo systems averaged over three replicates. The standard deviations were shown as filled area under curve. Residues 1-362 and 363-724 are cGAS monomer A and B, respectively.

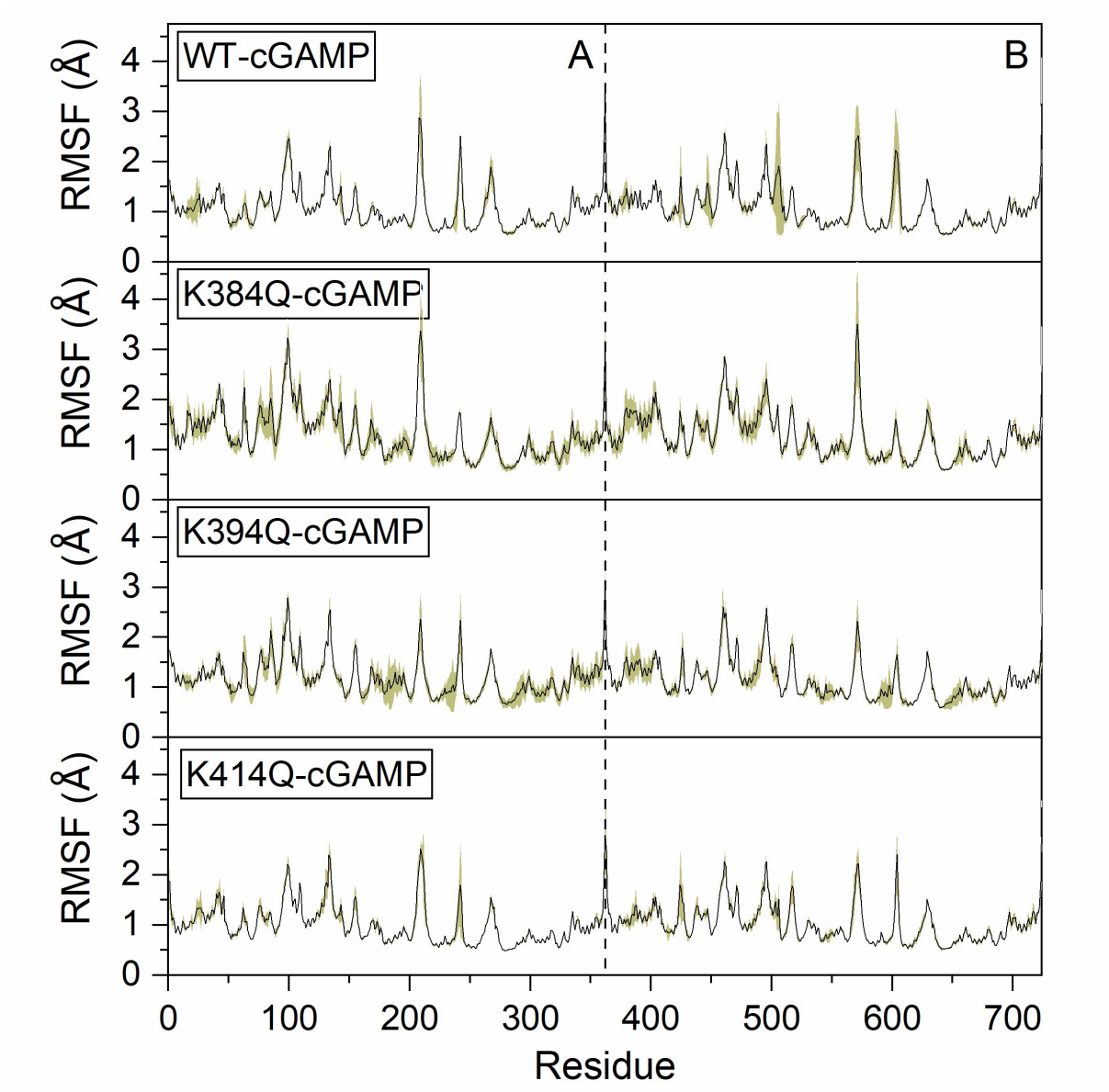

Fig. S6 The Cα root-mean-square fluctuations (RMSFs) of systems with cGAMP averaged over three replicates. The standard deviations were shown as filled area under curve. Residues 1-362 and 363-724 are cGAS monomer A and B, respectively.

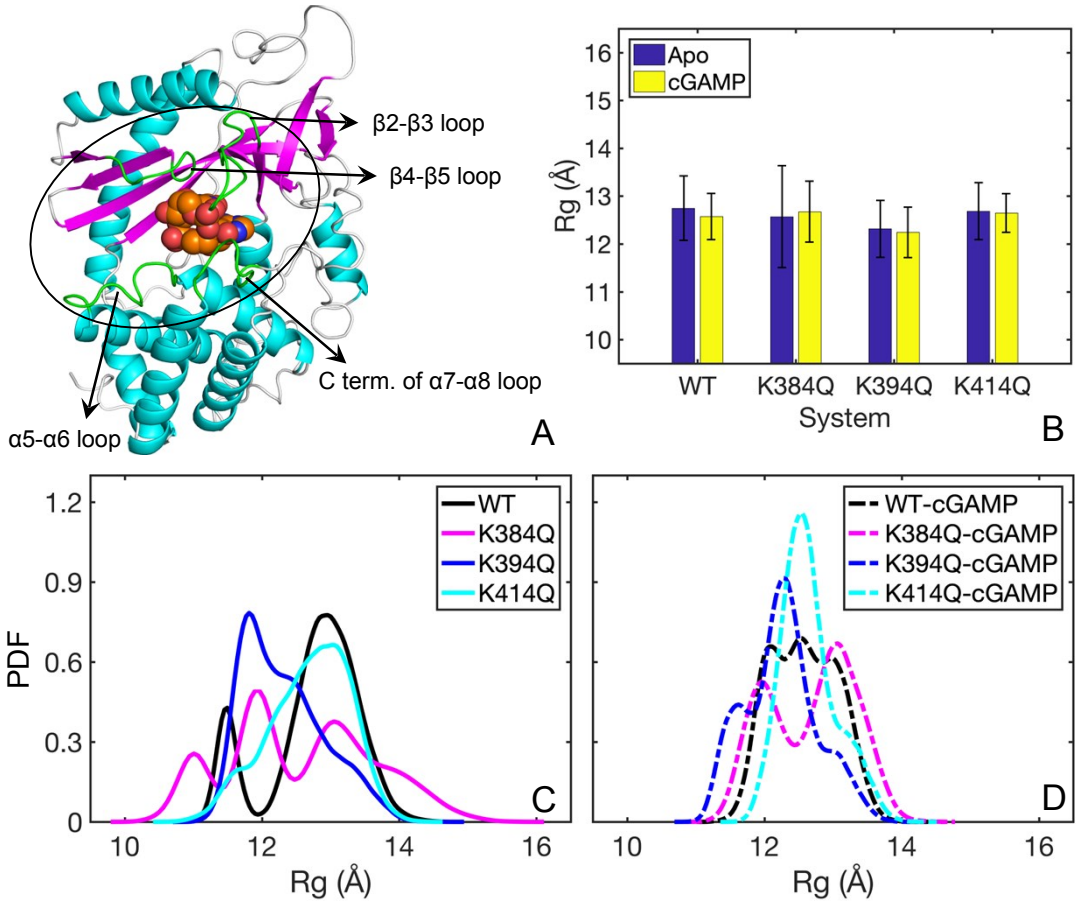

Fig. S7 The radius of gyration (R_g) of loops (the β2-β3, β4-β5, α5-α6 and the C-terminal of α5-α6 loops) around the active site during the last 100-ns simulations. (A) The cartoon model of cGAS with the active-site loops highlighted. The cGAMP was shown as spheres. (B) The average R_g of each system. (C-D) The probability distribution function (PDF) of the R_g in the absence and presence of cGAMP. The heavy atoms were considered here. Related to Fig. 6.

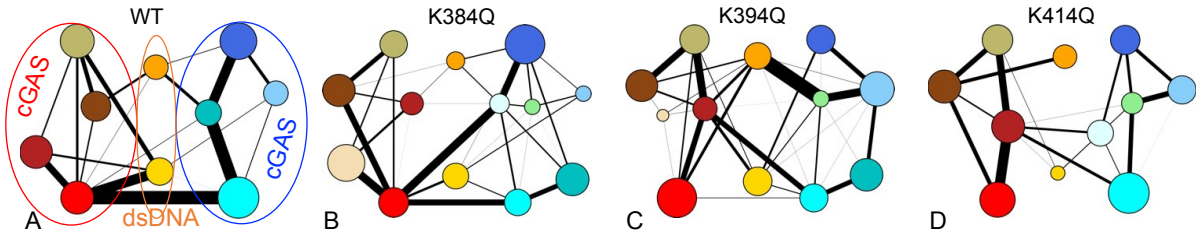

Fig. S8 Dynamical community analysis for apo cGAS-dsDNA dimer. Related to Fig. 7A-F.