

Supplementary Materials

Deciphering Conformational Changes of the GDP-Bound NRAS Induced by Mutations G13D, Q61R, and C118S through Gaussian Accelerated Molecular Dynamic Simulations

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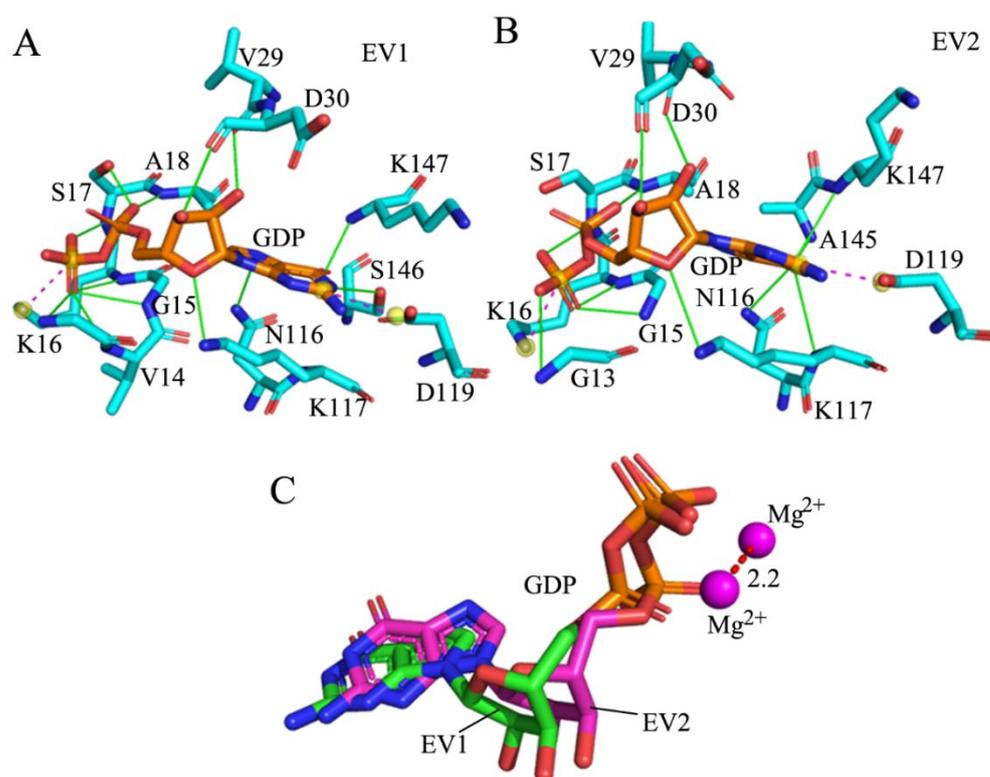


Figure S1. Interaction sites of GDP with NRAS and structural superimposition in the GDP-bound WT NRAS: (A) interaction sites of GDP with NRAS in the energetic state EV1, (B) interaction sites of GDP with NRAS in the energetic states EV2 and (C) structural superimposition of GDP and magnesium ions MG located at the EV1 and EV2.

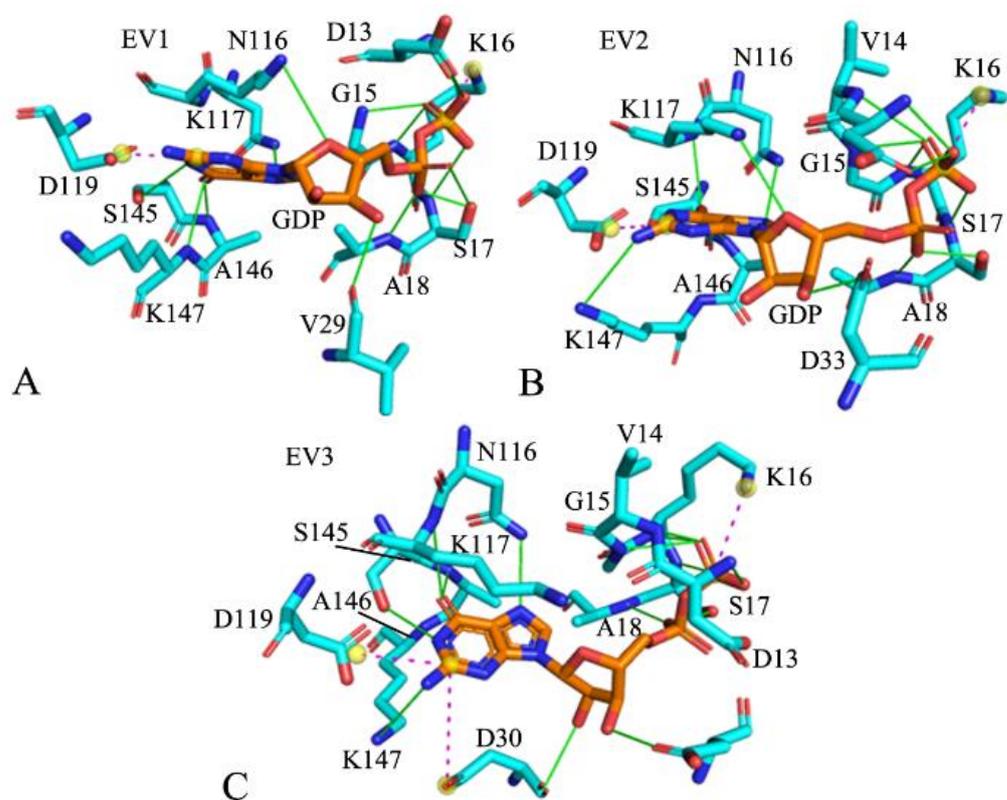


Figure S2. Interaction sites of GDP with NRAS in the GDP-bound G13D NRAS located at the different energetic states: (A) interaction sites of GDP with NRAS in the EV1, (B) interaction sites of GDP with NRAS in the EV2 and (C) interaction sites of GDP with NRAS in the EV3.

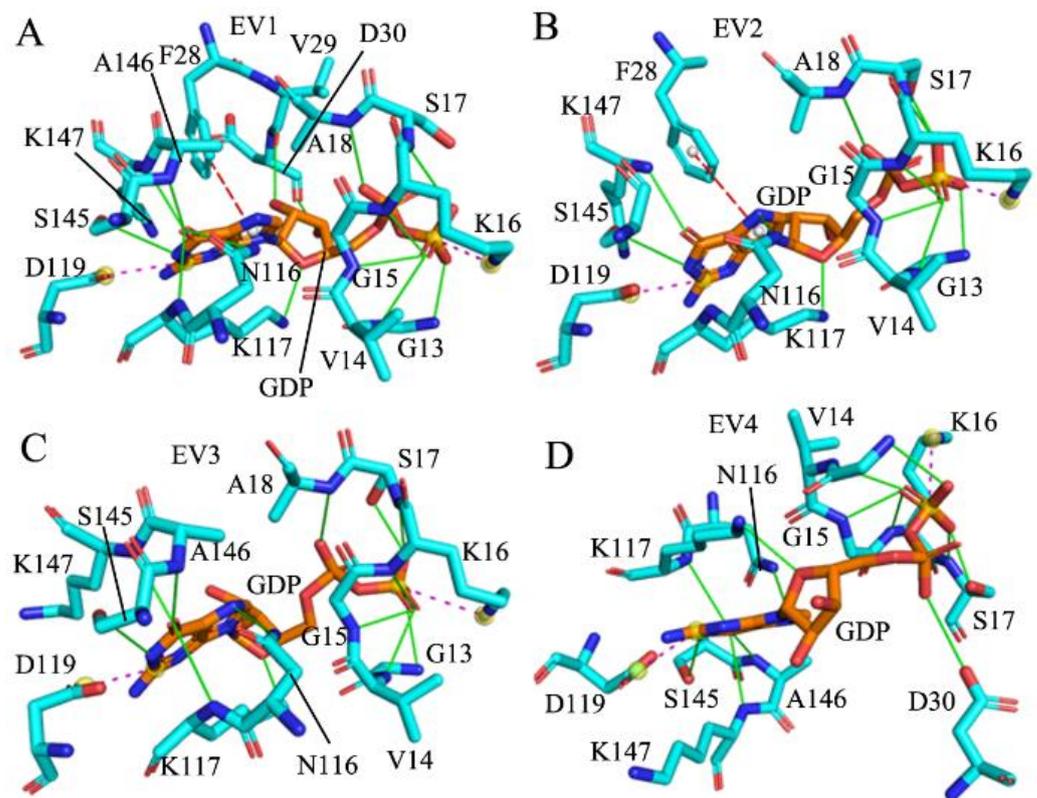


Figure S3. Interaction sites of GDP with NRAS in the GDP-bound Q61R NRAS located at the energetic states EV1-EV4: (A) interaction sites of GDP with NRAS in the EV1, (B) interaction sites of GDP with NRAS in the EV2, (C) interaction sites of GDP with NRAS in the EV3 and (D) interaction sites of GDP with NRAS in the EV4.

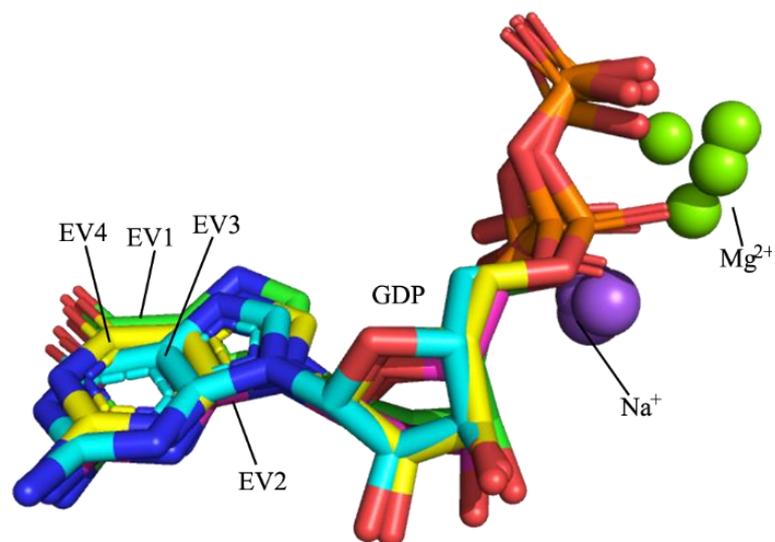


Figure S4. Superimposition of GDP and magnesium ions MG located at the energetic states EV1-EV4 of the GDP-bound Q61R NRAS.

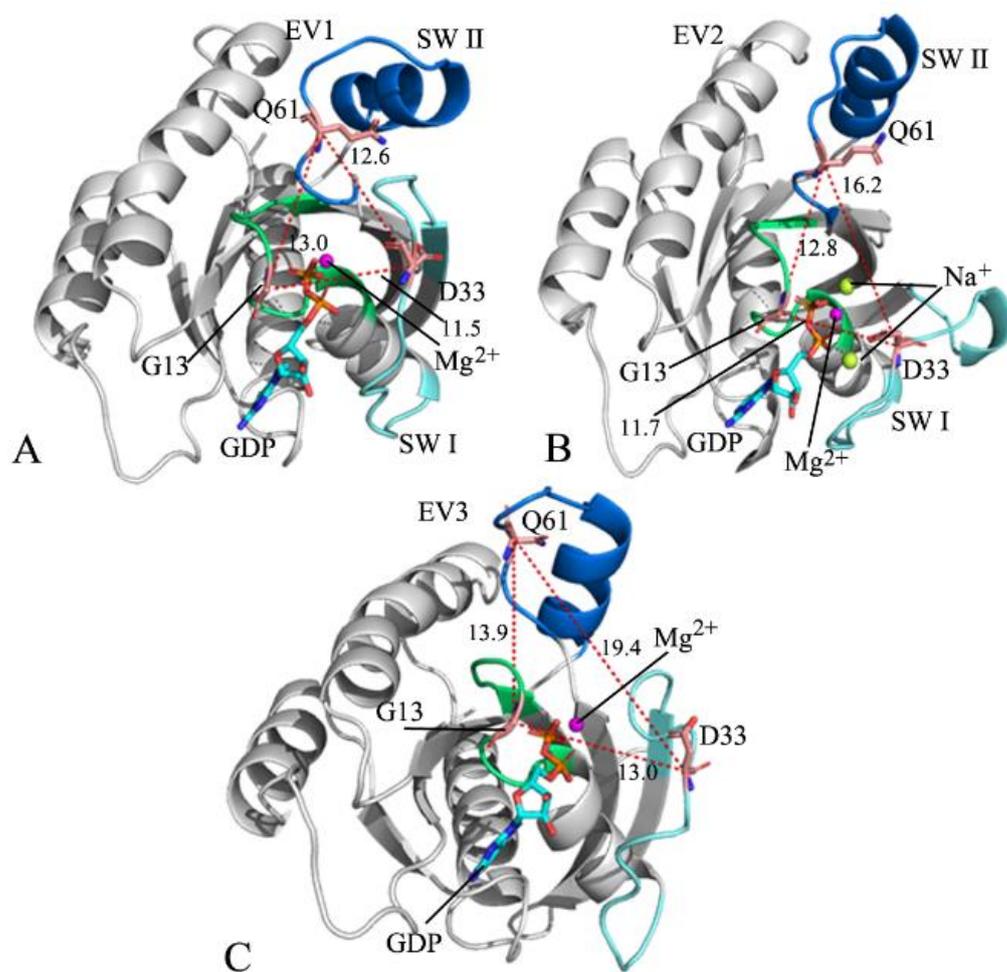


Figure S5. Representative structures of the GDP-bound C118S NRAS falling into the energy valleys EV1-EV3: (A) EV1, (B) EV2 and (C) EV3.

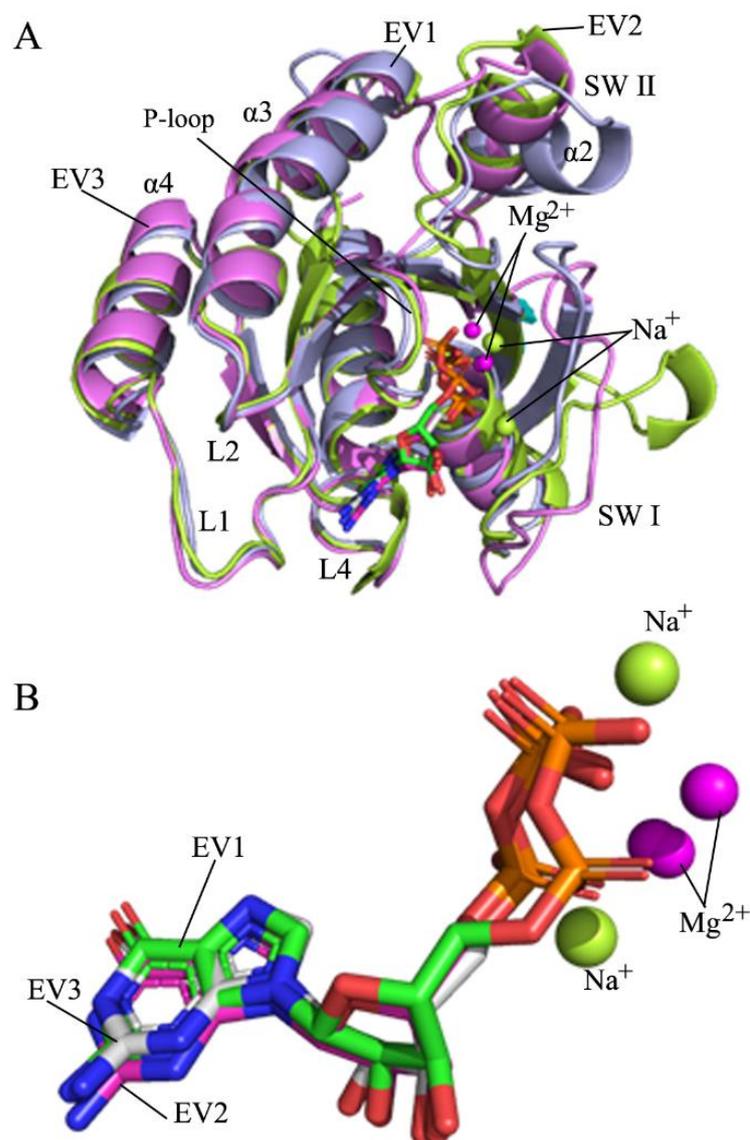


Figure S6. Superimposition of representative structures situated at the energy valleys EV1-EV3: (A) structural superimposition of the GDP-bound C118S NRAS and (B) structural superimposition of GDP and magnesium ions MG.

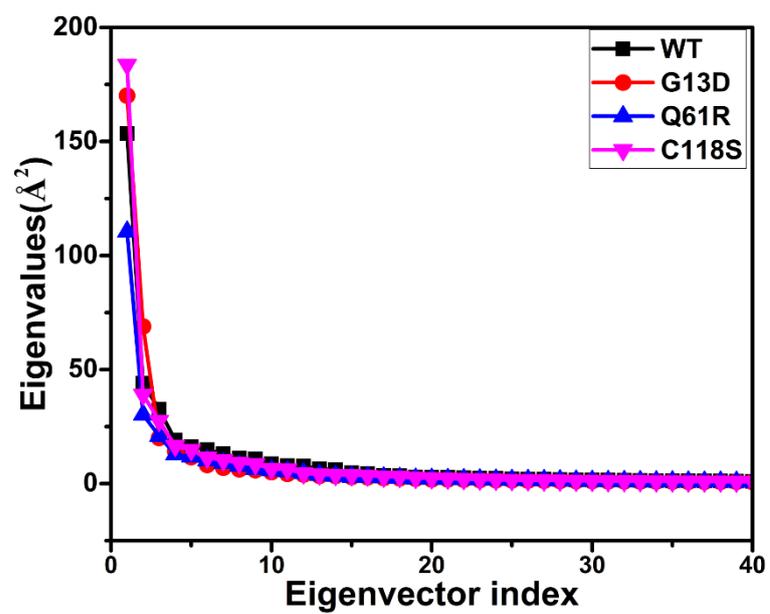


Figure S7. Function of eigenvalues VS eigenvector indexes from principal component analysis, which is used to describe motion intensity of NRAS.