Phosphorylation Mechanism of N-acetyl-L-Glutamate Kinase, a QM/MM Study

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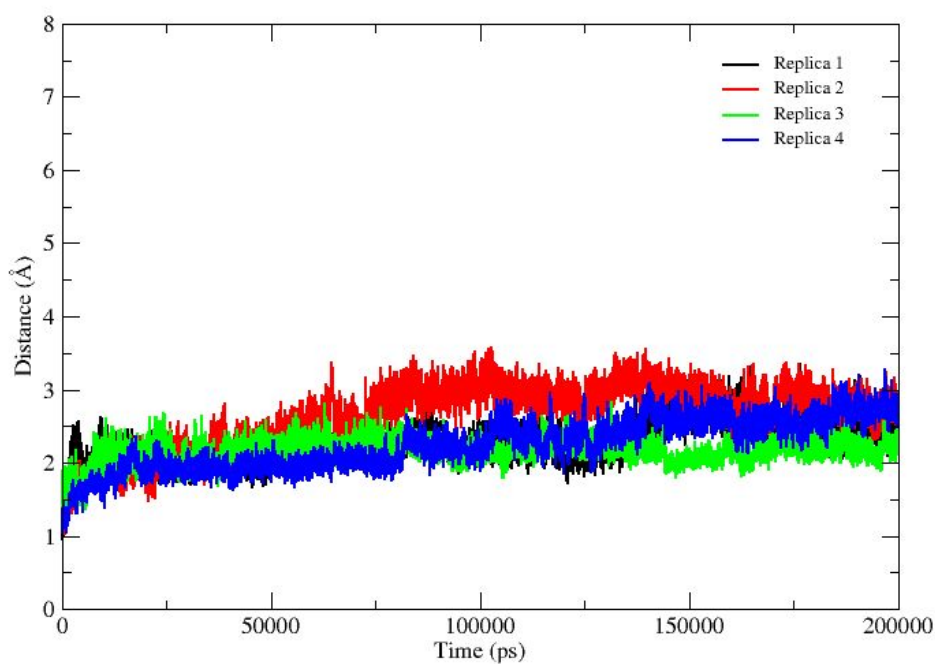
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Table S1. RESP charges of atoms in NAGK.

No.	Atom name	Atom type	RESP Charge
1	C1	CT	0.21
2	C2	C	0.85
3	C3	CT	0.04
4	C4	CT	-0.23
5	C5	C	0.75
6	C6	C	0.96
7	C7	CT	-0.57
8	O1	O2	-0.82
9	O2	O2	-0.82
10	O3	O	-0.58
11	O4	OH	-0.60
12	O5	O	-0.70
13	N1	N	-0.80
14	H1	H1	0.08
15	H2	HC	-0.01
16	H3	HC	-0.01
17	H4	HC	0.06
18	H5	HC	0.06
19	H6	HC	0.14
20	H7	HC	0.14
21	H8	HC	0.14
22	H9	H	0.34
23	H10	HO	0.40
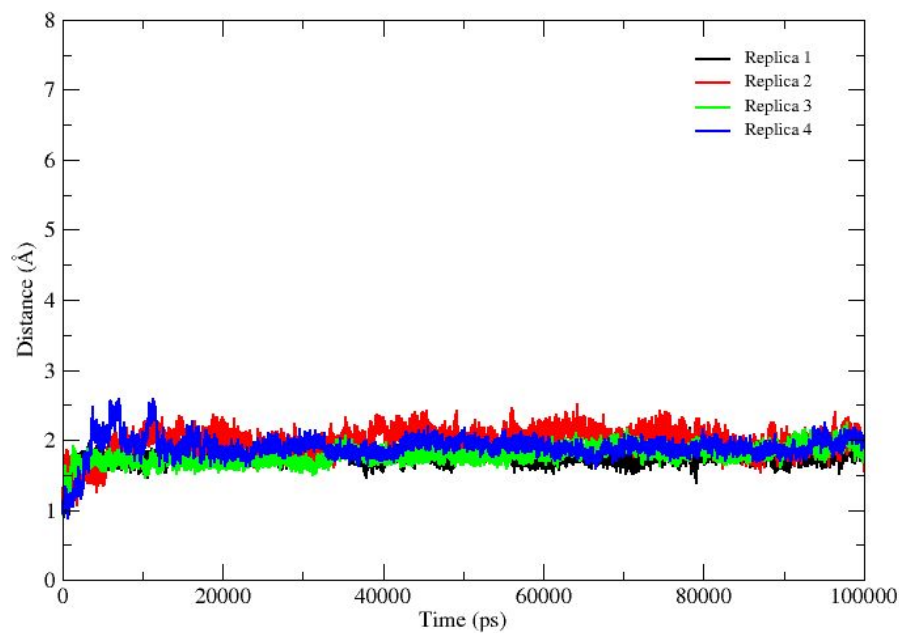
(a)

(b)

Figure S1. (a) RMSD values for Cα carbon of the backbone of ATP -Mg^{2+}-NAGK-NAG complex (b) RMSD values for Cα carbon of the backbone of ATP-Mg^{2+}-NAGK complex.
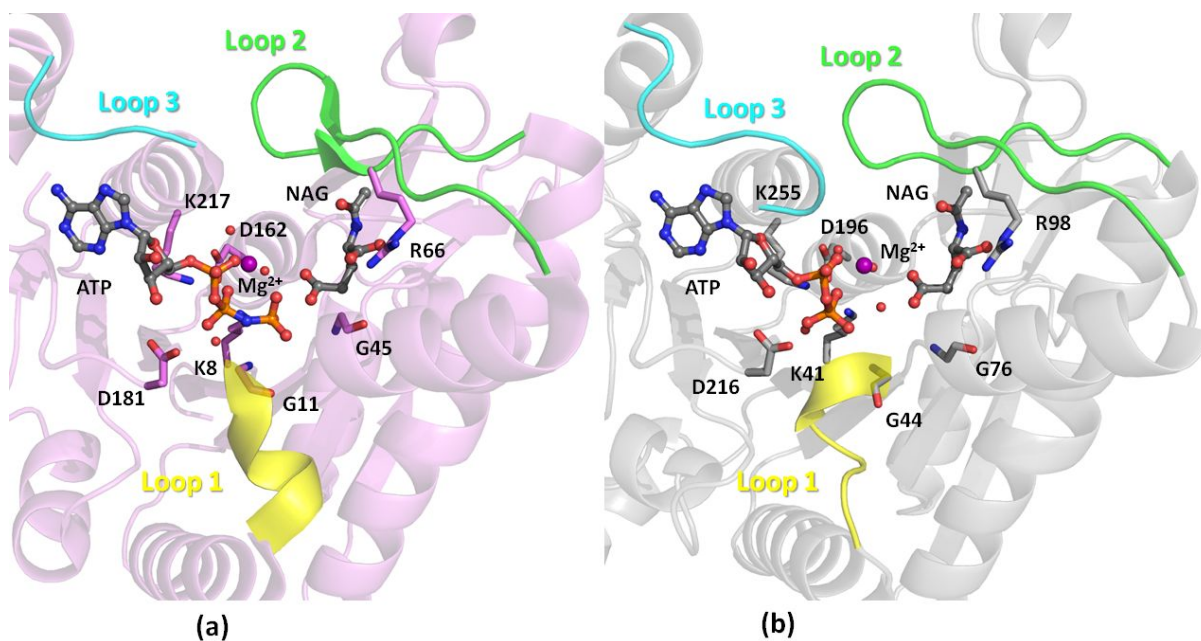
Figure S2. Comparison of *E. Coli* NAGK and *A. Thaliana* NAGK (a) Crystal structure of *Escherichia coli* NAGK (Ec-NAGK) in complex with AMPPNP, Mg^{2+} and NAG (PDB Code: 1GS5) (b) Crystal structure of *Arabidopsis thaliana* NAGK (At-NAGK) in complex with ADP, Mg^{2+} and NAG (PDB Code: 4USJ).
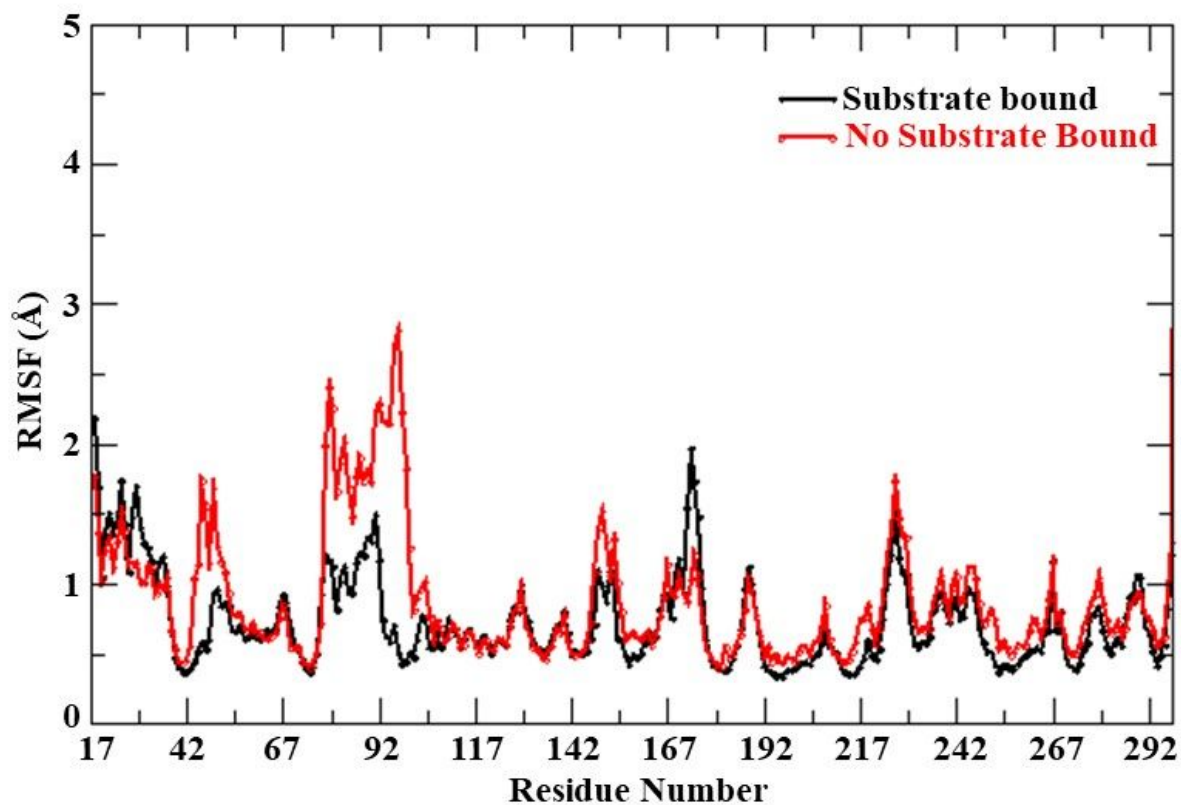
Figure S3. The RMSF analysis of NAGK. The residues represented in the black illustrate the ATP -Mg^{2+}-NAGK-NAG complex. Those represented in red represent the ATP-Mg^{2+}-NAGK complex.
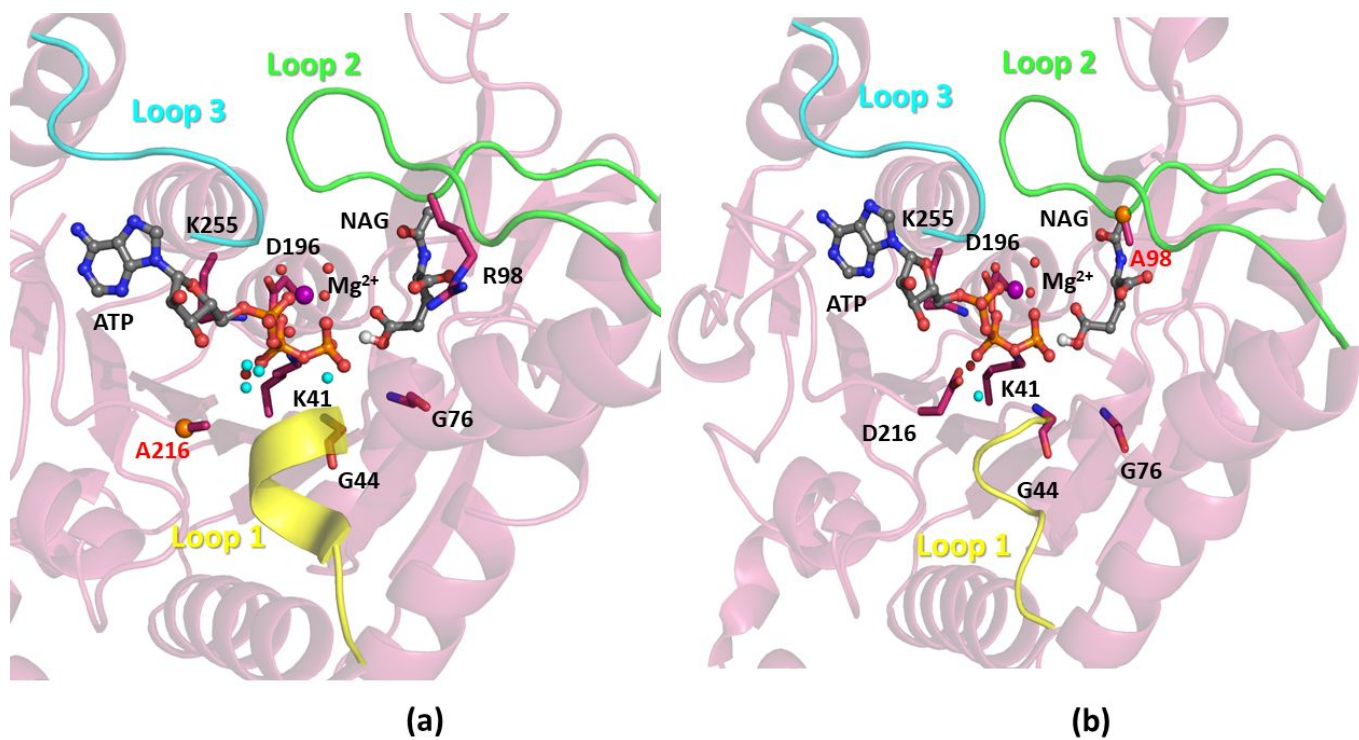
Figure S4. Representative structures of At-NAGK mutants from MD simulations (a) D216A

(b) R98A. Loop 1, 2 and 3 are highlighted in yellow, green and cyan respectively.