Supplementary Material (ESI) for PCCP

Electronic Supplementary Information

Theoretical Study of the Opsin Shift of Deprotonated Retinal Schiff Base in a Bacteriorhodopsin Environment

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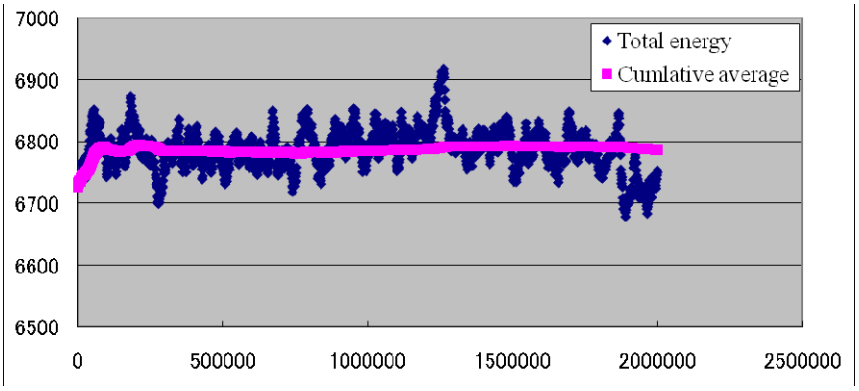
S1. Total energy, temperature, and pressure along the classical molecular dynamics trajectory

After the NVT ensemble MD calculation with T = 300 K for 100 ps, we performed NPT ensemble MD calculations with T = 300 K and P = 1.0 atm for 2 ns. The data for the first 1 ns was used for the equilibration. The next 1 ns was used to obtain thermodynamic quantity. In the followings, we show total energy, temperature, pressure and their cumulative average during the MD simulation. The snapshots were taken from the last 0.5 ns.

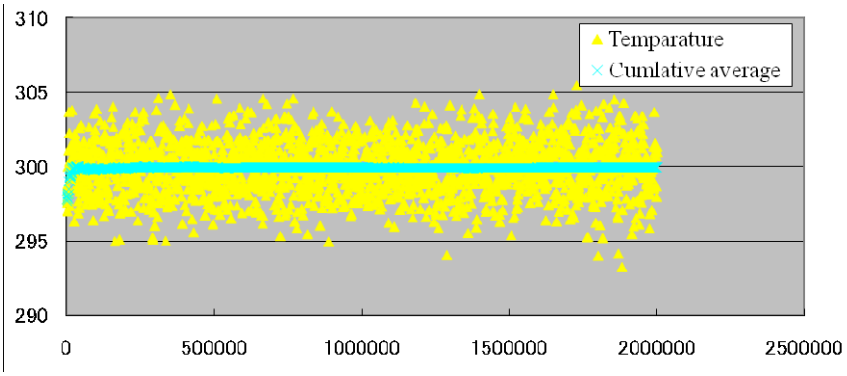
(1) Total energy:

Average over 2000000 steps = 6787.0506 kcal/mol



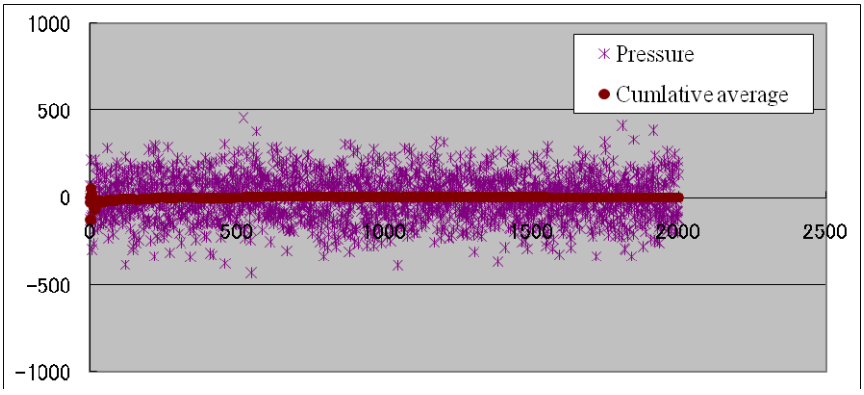
(2) Temperature

Average over 2000000 steps = 299.88 K



(3) Pressure

Average over 2000000 steps = 299.88 K = 1.1 atm



S2. List of protonation states of the charged amino acids in bR.

List of the protonation states of the charged amino acids were summarized in Table S1. Asp85 in the M state is protonated because the proton was just transferred from the retinal chromophore.[1] Asp96 was also protonated because the DPSB accept a proton from Asp96 in the next step.[2, 3] Because the 1M0M[4] and 1CWQ[5] structures are regarded as those before and after the proton release to the extracellular side, respectively, Glu204 was protonated and deprotonated in the models B and A, respectively. Aspartates and glutamates in the protein surface were protonated because counter ions can neutralize the charges. Arginines and lysines in the surface were associated with the chloride ions. Total charges of the models B and A are 0 and -1, respectively.

Table S1 List of protonation states of the charged residues.

Charged residues	Residue ID	Model B Before PT	Model A After PT
ARG	7	1	1
GLU	9	-1	-1
LYS	30	0	0
ASP	36	-1	-1
ASP	38	-1	-1
LYS	40	1	1
LYS	41	1	1
GLU	74	0	0
ARG	82	1	1
ASP	85	0	0
ASP	96	0	0
ASP	102	0	0
ASP	104	0	0
ASP	115	0	0
LYS	129	0	0
ARG	134	1	1
LYS	159	1	1
GLU	161	-1	-1
ARG	164	1	1
GLU	166	-1	-1
LYS	172	0	0
ARG	175	0	0
GLU	194	-1	-1
GLU	204	0	-1
ASP	212	-1	-1
RET	216	0	0
ARG	225	0	0
ARG	227	0	0

References

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