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

Zinc Ion-Induced Conformational Changes of New Delphi Metallo-β-lactamase 1 Probed by Molecular dynamics Simulations and Umbrella Sampling

Jianzhong Chen[a,*], Jinan Wang[b,*] and Weiliang Zhu[b]

[a]School of Science, Shandong Jiaotong University, Jinan, 250014, China.

E-mail: chenjianzhong1970@163.com and jzchen1970@126.com;

[b]Drug Discovery and Design Center, CAS Key Laboratory of Receptor Research, Shanghai Institute of Materia Medica, Chinese Academy of Sciences, 555 Zuchongzhi Road, Shanghai, 201203, China.

E-mail: jawang@simm.ac.cn

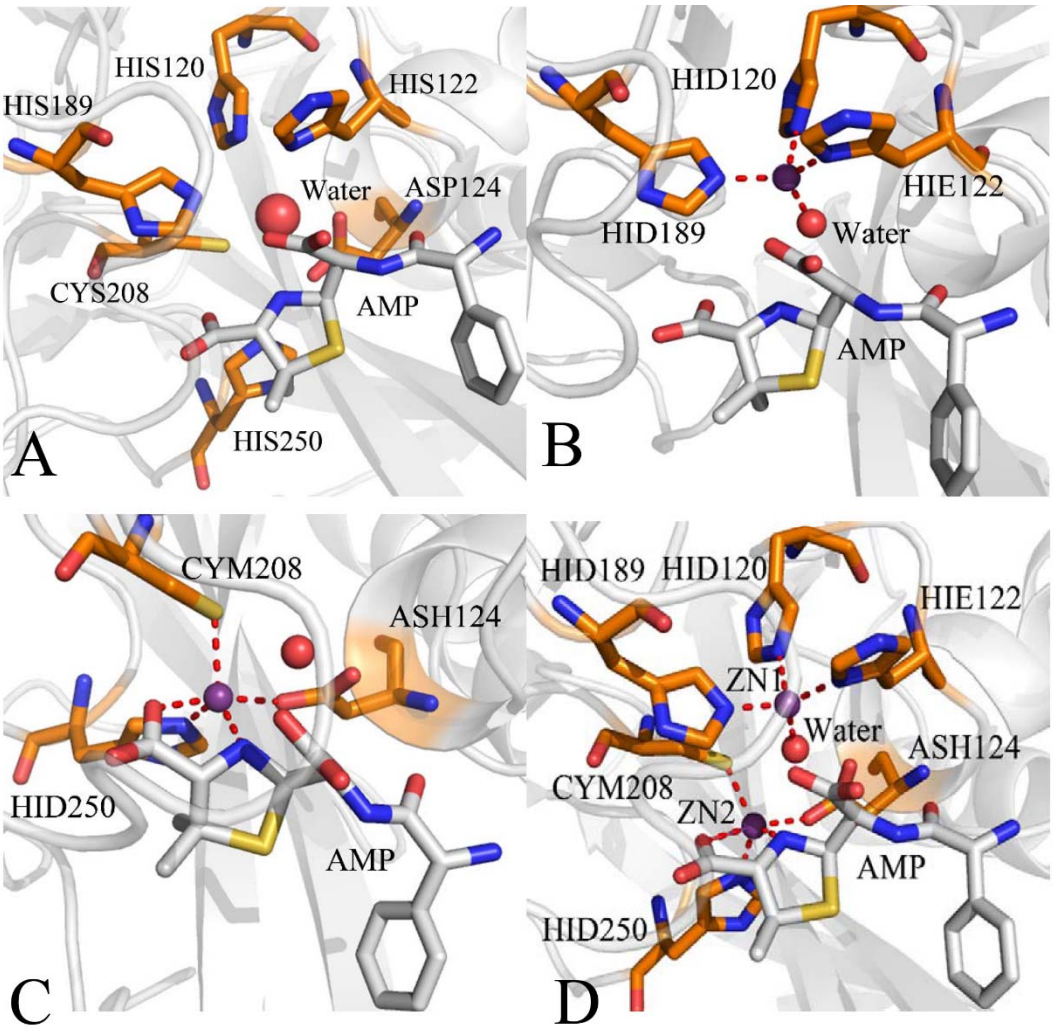

Fig. S1 Four models involved in the current work: (A) without zinc ions, (B) geometry of Zn1 coordination, (C) geometry of Zn2 coordination and (D) geometry of double-Zn coordination.

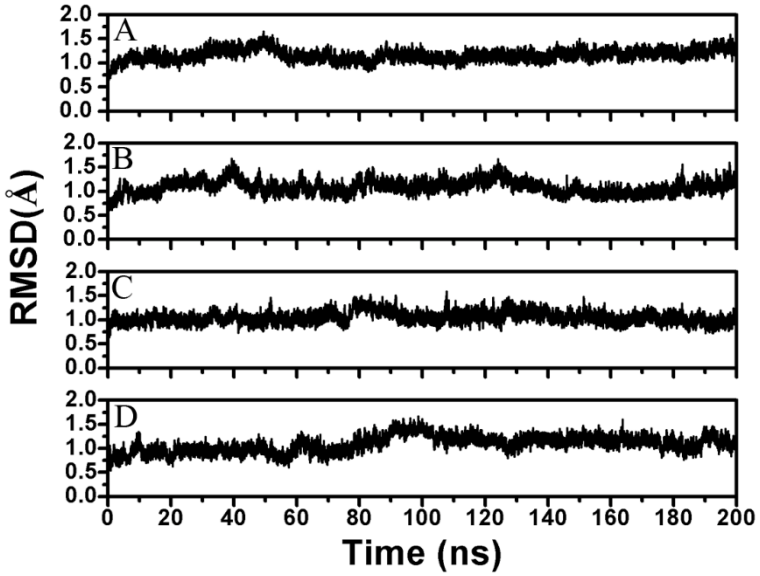

Fig. S2 Root-mean-square deviation (RMSD) of backbone atoms in NDM-1 relative to the crystal structure as a function of simulation time: (A) without zinc ions, (B) geometry of Zn1 coordination, (C) geometry of Zn2 coordination and (D) geometry of double-Zn coordination.

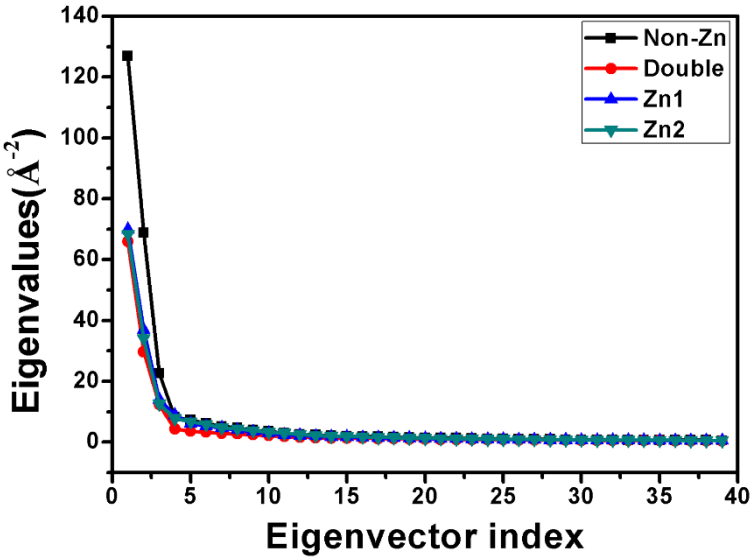

Fig. S3 Eigenvalues plotted against the corresponding eigenvectors indices stemming from principal component analysis.

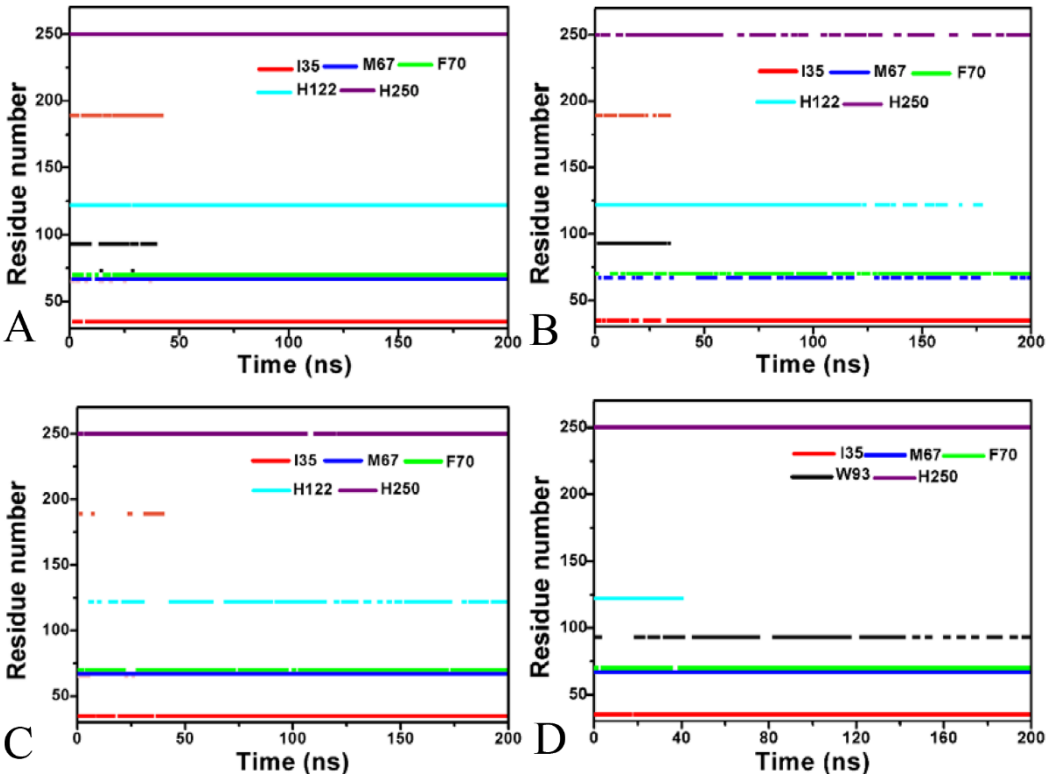

Fig. S4. The hydrophobic contacts of AMP with residues of NDM-1 as a function of simulation time, (A) double-Zn coordination model, (B) without zinc ions, (C) only Zn1 coordination model and (D) only Zn2 coordination model.

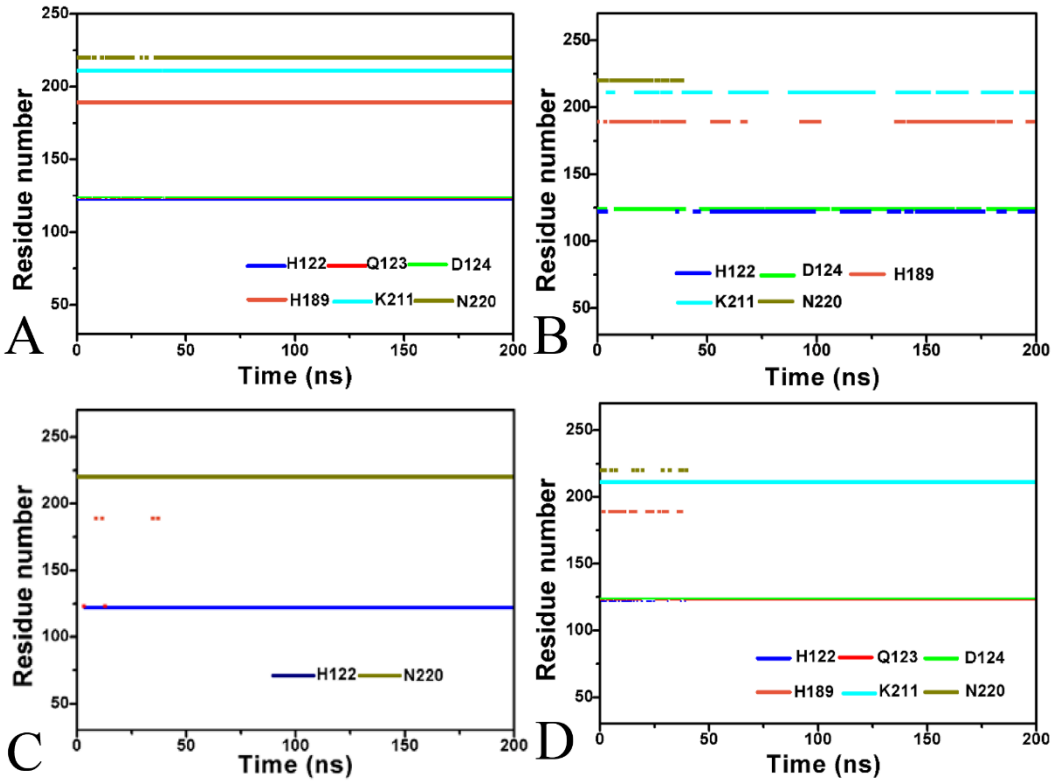

Fig. S5 The hydrogen bond contacts formed between AMP and residues of NDM-1 as a function of simulation time, (A) double-Zn coordination model, (B) Without zinc ions, (C) only Zn1 coordination model and (D) only Zn2 coordination model.

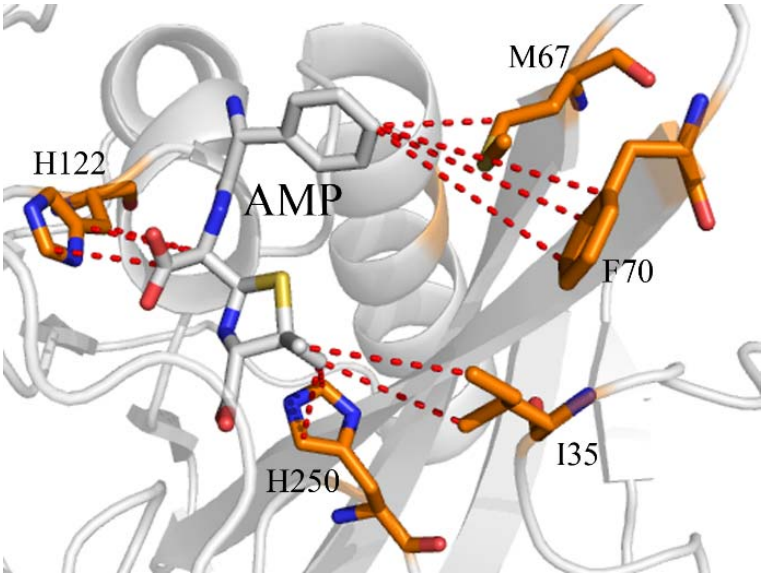

Fig. S6 Residues of NDM-1 forming hydrophobic contacts with AMP. Key residues and AMP are displayed in stick modes. A pair of carbon atoms lower than 4.2 Å in distances are thought to form hydrophobic interactions.

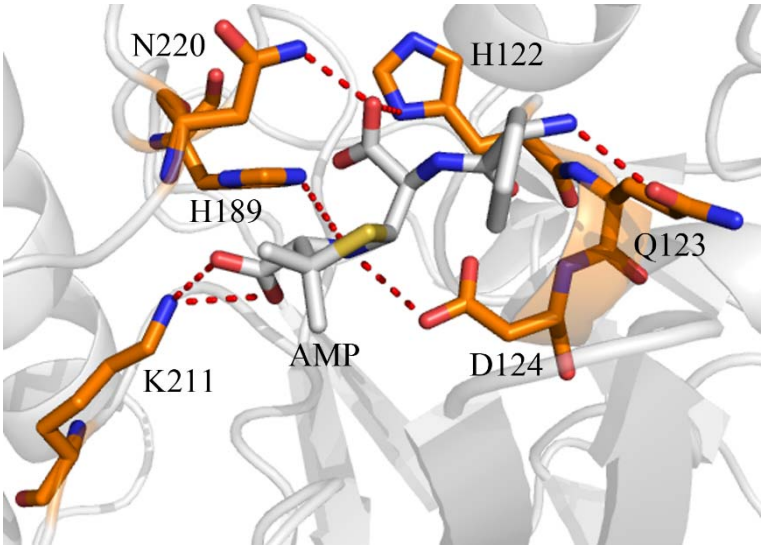

Fig. S7 Hydrogen bonds between AMP and NDM-1 detected by hydrogen bond scanning, Key residues and AMP were displayed in stick modes.

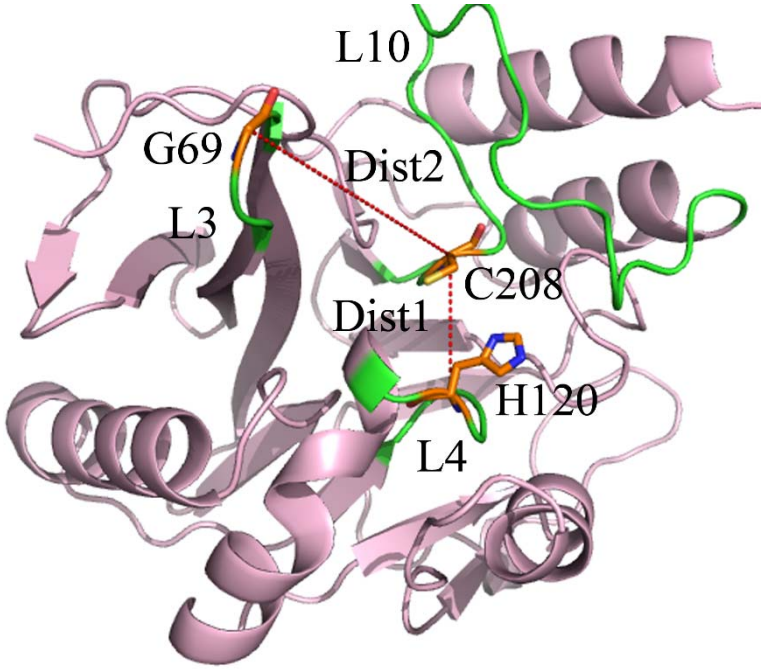

Fig. S8 Definition of reaction coordinate: Dist1 represents the distance between two C_α atoms of residues H120 and C208 and Dist2 indicates the distance between two atoms of residues G69 and C208. NDM-1 is displayed in cartoon modes, residues G69, H120 and C208 are described in stick modes and three loops are represented by green color.