

**Molecular Mechanism and Energy Basis of Conformational Diversity of Antibody
SPE7 Revealed by Molecular Dynamics Simulation and Principal Component
Analysis**

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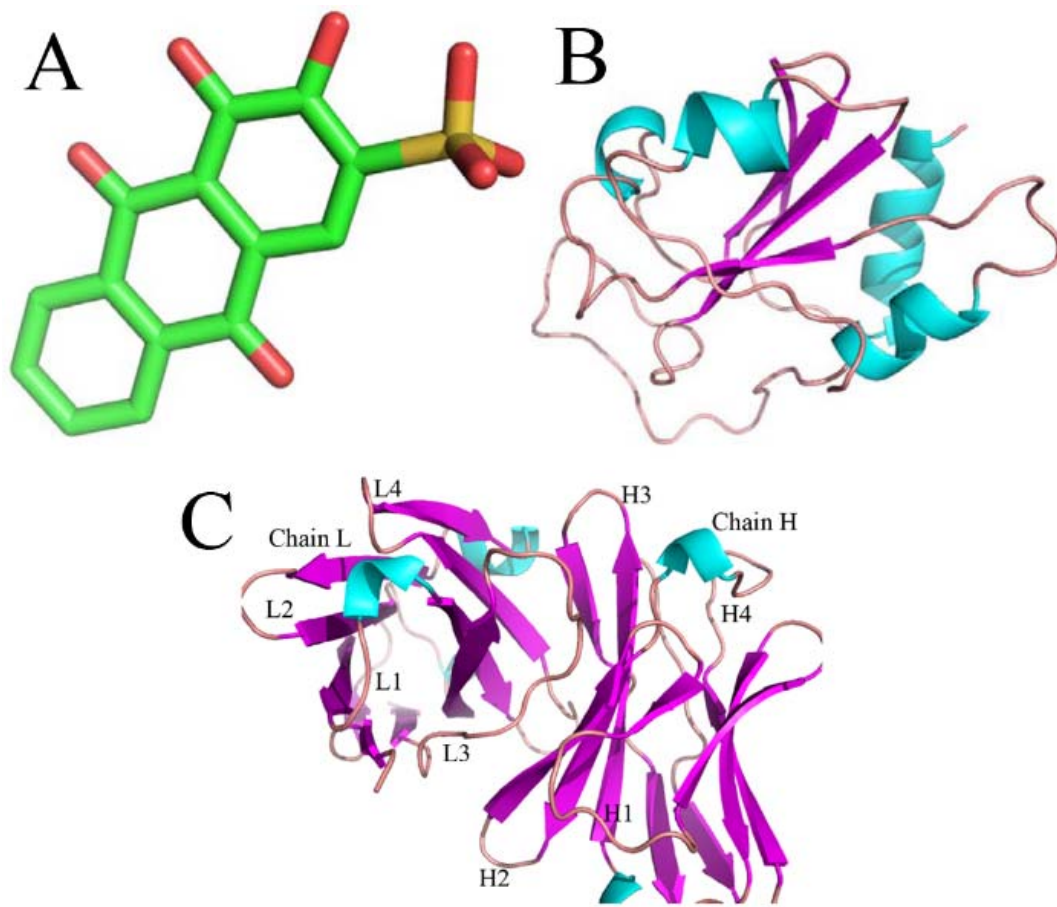


Figure S1 structures of AZR, antigens Trx-Shear3 and antibody SPE7: (A) AZR, (B) Trx-Shear3 and (C) antibody SPE7.

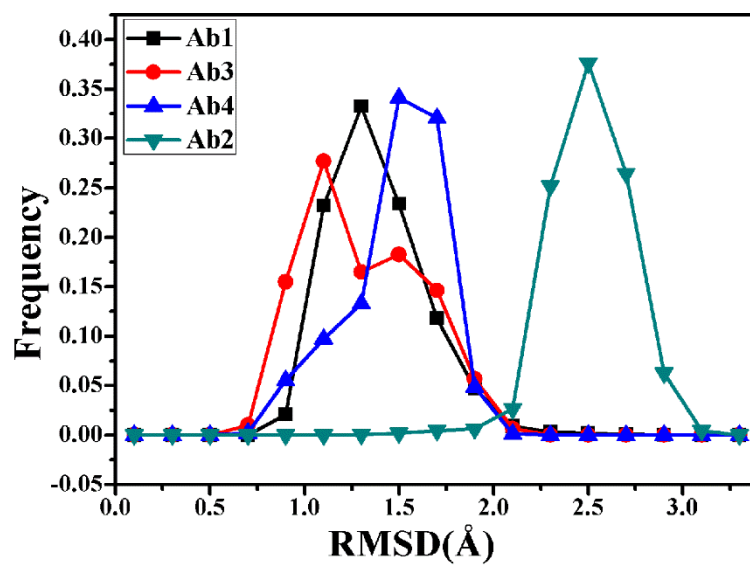


Figure S2 Frequency distribution of root-mean-square deviations (RMSD) of the backbone atoms relative to the corresponding crystal structures

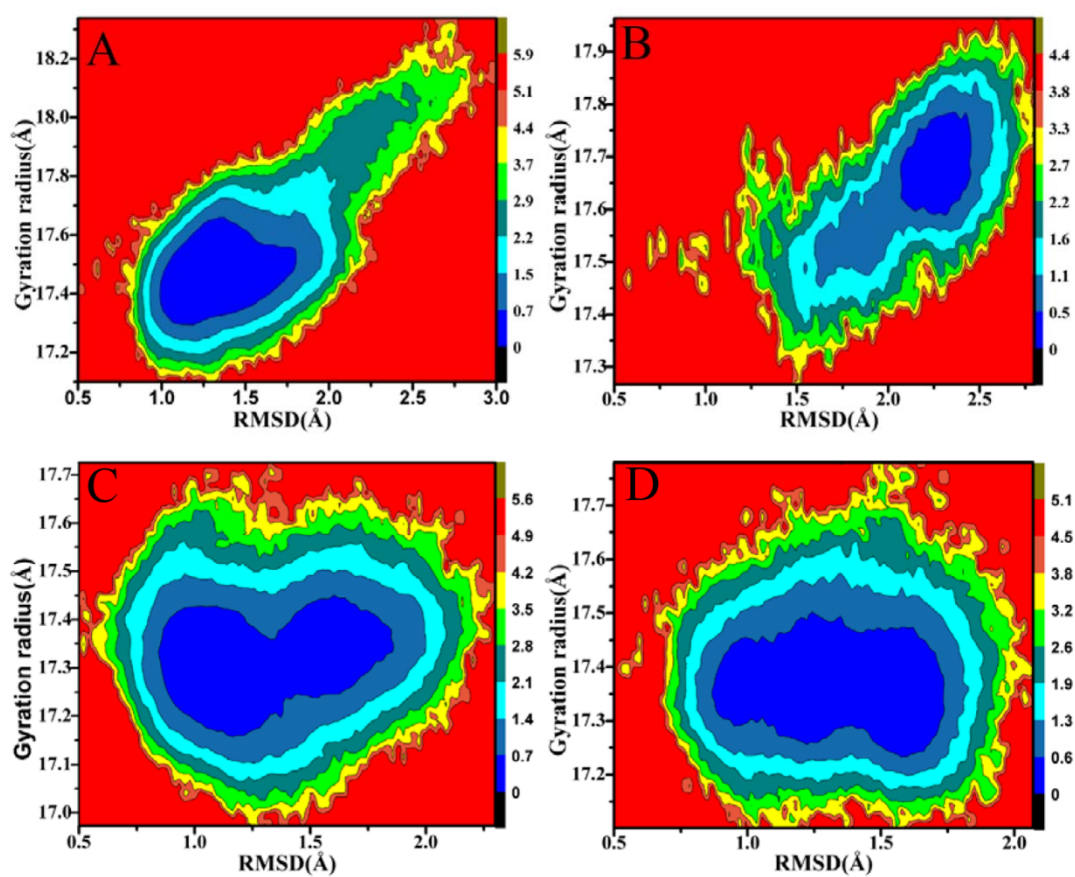


Figure S3 Free energy landscape of four different conformations Ab1, Ab2, Ab3 and Ab4 built by using RMSD and gyration radius: (A) Ab1, (B) Ab2, (C) Ab3 and (D) Ab4.

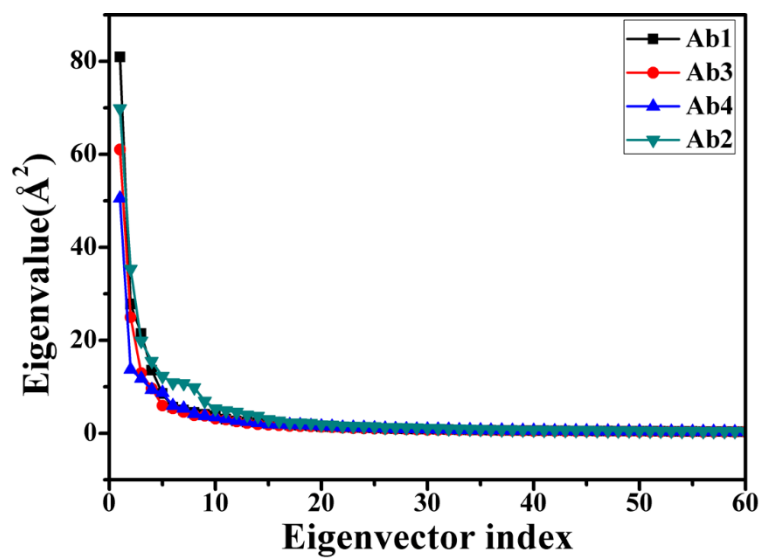


Figure S4 Comparison of the eigenvalues plotted against the corresponding eigenvectors indices obtained from the C_{α} covariance matrix built from MD trajectories.

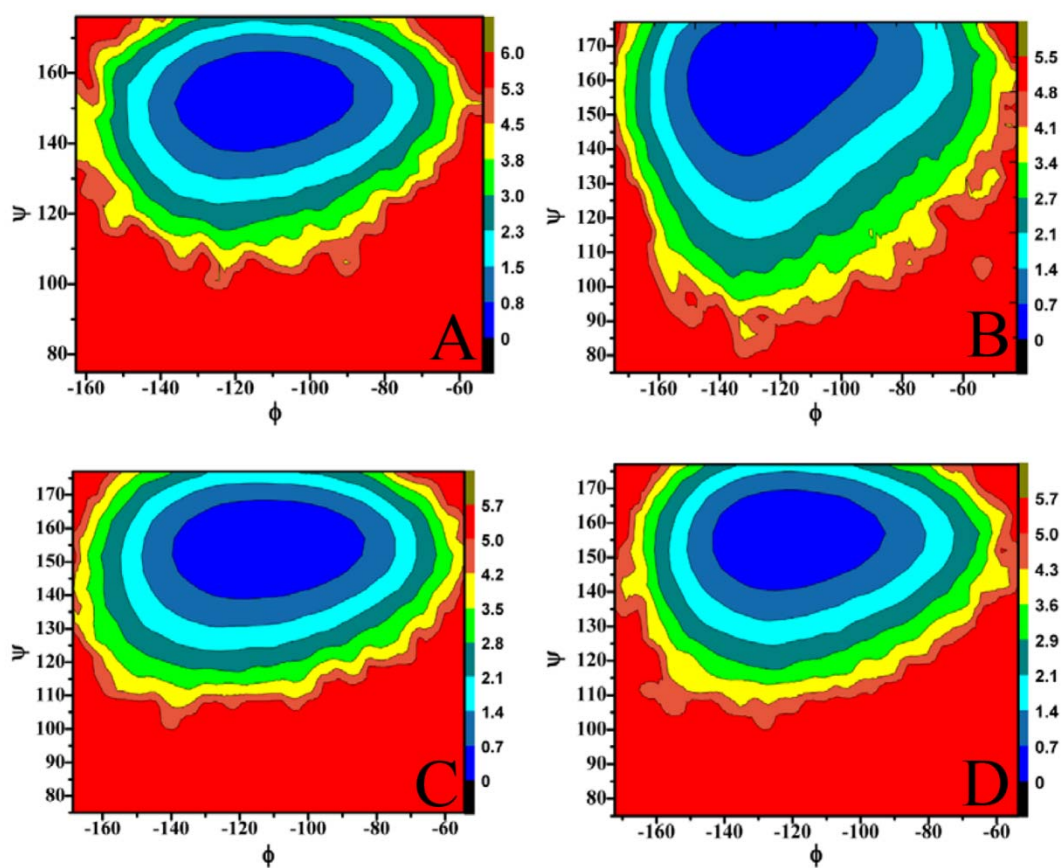


Figure S5 Energy landscapes constructed by using the backbone angle of the residue H-W33: (A) Ab1, (B) Ab2, (C) Ab3 and (D) Ab4.

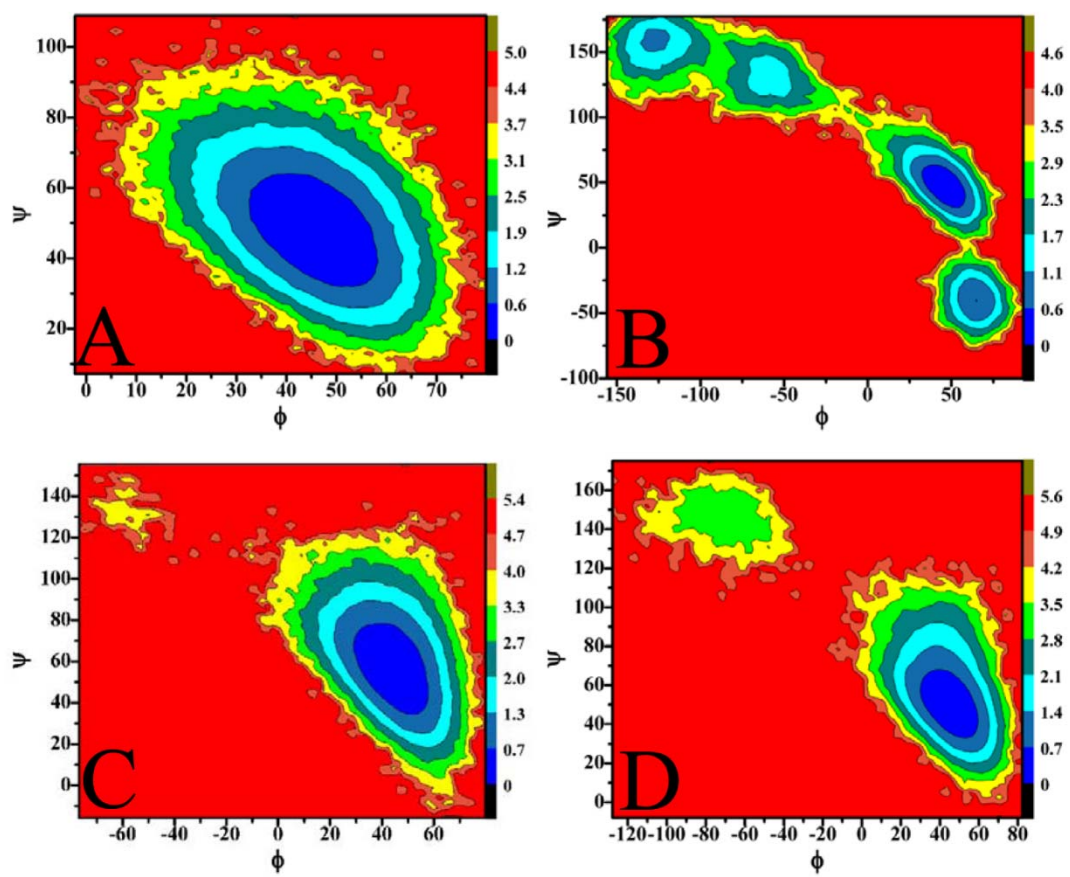


Figure S6 Energy landscapes constructed by using the backbone angle of the residue L-Y34: (A) Ab1, (B) Ab2, (C) Ab3 and (D) Ab4.

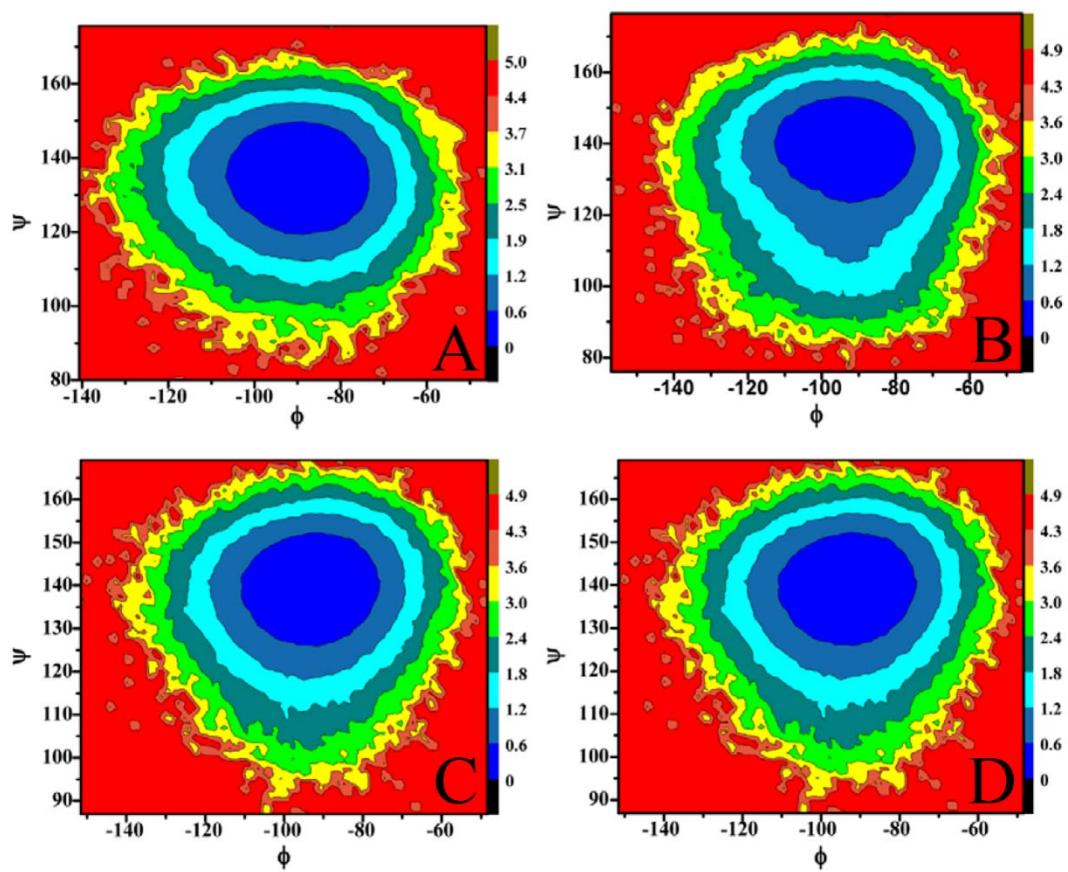


Figure S7 Energy landscapes constructed by using the backbone angle of the residue H-W33: (A) Ab1, (B) Ab2, (C) Ab3 and (D) Ab4.

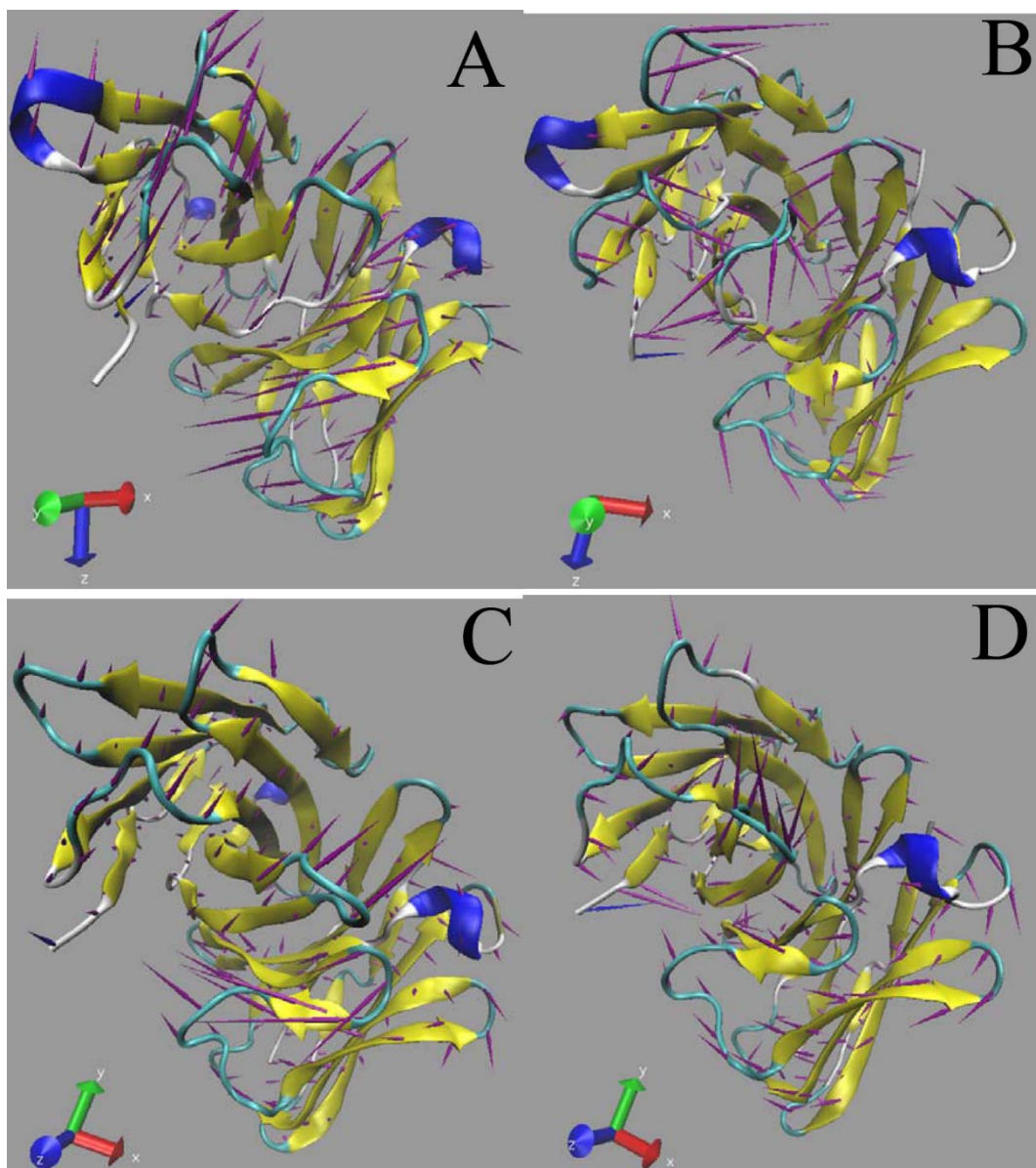


Figure S8 Porcupine plot corresponding to PC1 obtained by performing principal component analysis on new MD trajectories: (A) Ab1, (B) Ab2, (C) Ab3 and (D) Ab4.

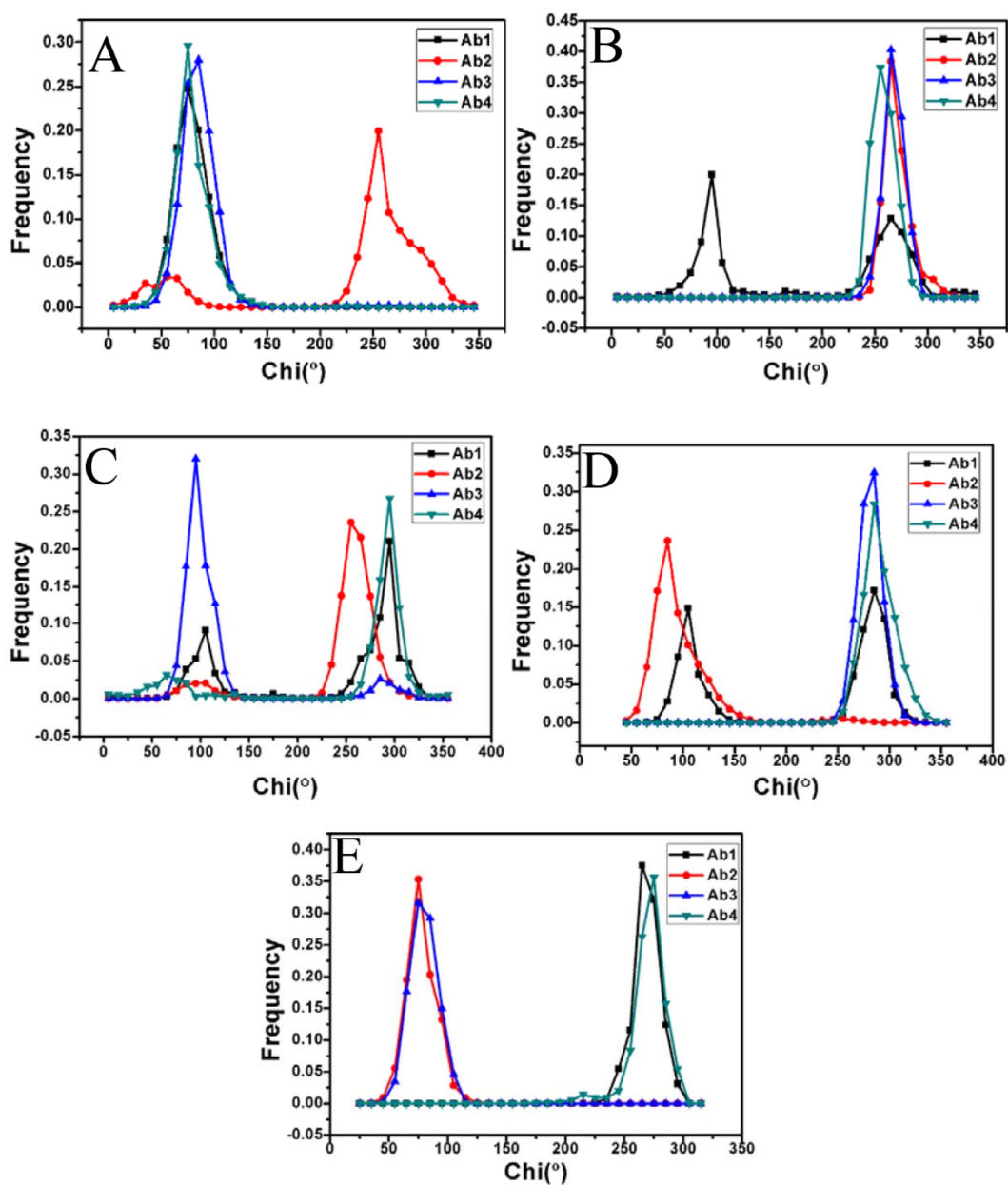


Figure S9 Frequency distribution of dihedral angle by using new MD trajectories: (A) H-W33, (B) H-Y101, (C) H-Y105, (D) L-Y34 and (E) L-W93.