Stability determination of Protein Data Bank structures

Osaka University, Institute for Protein Research

Purpose: Stability determination of Protein Data Bank (PDB) structures

- Outline: High temperature molecular dynamics (MD) simulations (400 K) can be used as an effective tool to evaluate the stability of proteins. The Dynamics DataBank (DDB) (https://bsma.pdbj.org/dynamicsdb/) includes the stability analysis of a large number of single-chained PDB entries. To expand the dataset, we selected several multi-chained PDB entries, and we used the CMC SQUID cluster to perform similar simulations.
- **Result** For 27 multi-chained PDB entries, we performed 10 x 100ns canonical MD simulations at 400 K. After analysis these will be added to the DDB.

Computing system: node-hour:

SQUID GPGPU nodes 3800 NH

