**S1 Table.** Energy and radius of gyration values for apo and holo crystal structures

|  |  |  |
| --- | --- | --- |
| Protein | Minimization energya(kcal/mol) | Radius of gyration- RG*b* (Å)  |
| apo | Holo | apo | holo | predicted*c* |
| AK | -7065 | -7115 | 19.4 | 16.4 | 16.9 |
| BC | -27764 | -27652 | 23.2 | 21.7 | 22.3 |
| LAO | -6826 | -6853 | 19.1 | 17.7 | 17.6 |
| DBP | -14840 | -14742 | 24.7 | 22.8 | 23.5 |
| CAM | -5685 | -5710 | 20.3 | 16.5 | 14.7 |

*a* The energy value obtained at the end of minimization in implicit solvent. The details of the minimization are given in Methods. The energy of the holo state is calculated without the ligand.

*b*RG is calculated using VMD, according to following formula:

$RG=\sqrt{\left(\sum\_{i=1}^{n}w(i)(r\left(i\right)-\overbar{r})^{2}\right)/\left(\sum\_{i}^{n}w(i)\right)}$

where *w(i)* and *r(i)* are the mass and the position of ith atom, respectively and $\overbar{r}$ is the center of mass.

*c*RG of monomeric proteins (*N* residues long) can be predicted using the empirical equation by Kolinski and Skolnick (1):

$RG=2.2 N^{0.38}$

**Reference**

1. Kolinski A, Skolnick J. Monte Carlo simulations of protein folding. I. Lattice model and interaction scheme. Proteins. 1994;18(4):338–52.