Ligand-Free Open–Closed Transitions of Periplasmic Binding Proteins: the Case of Glutamine-Binding Protein

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Supporting Information

Table S1. Q-factor Statistics for PRE Fit Performed via Optimization of the Paramagnetic Probe Side Chain Represented by a Six-Conformer Ensemble.[a]

	overall	intradomain	interdomain
unliganded S51C	0.22 ± 0.02	0.20 ± 0.02	0.43 ± 0.00
liganded S51C	0.21 ± 0.00	0.23 ± 0.00	0.19 ± 0.00
unliganded D122C	0.20 ± 0.01	0.17 ± 0.02	0.43 ± 0.01
liganded D122C	0.27 ± 0.01	0.28 ± 0.02	0.25 ± 0.02

[a] The optimization procedure replicates exactly that described in the Article, except for the number of conformers used to represent the probe. Statistics exclude residues 143–149, 168, 169, and 173 (see Article for details).

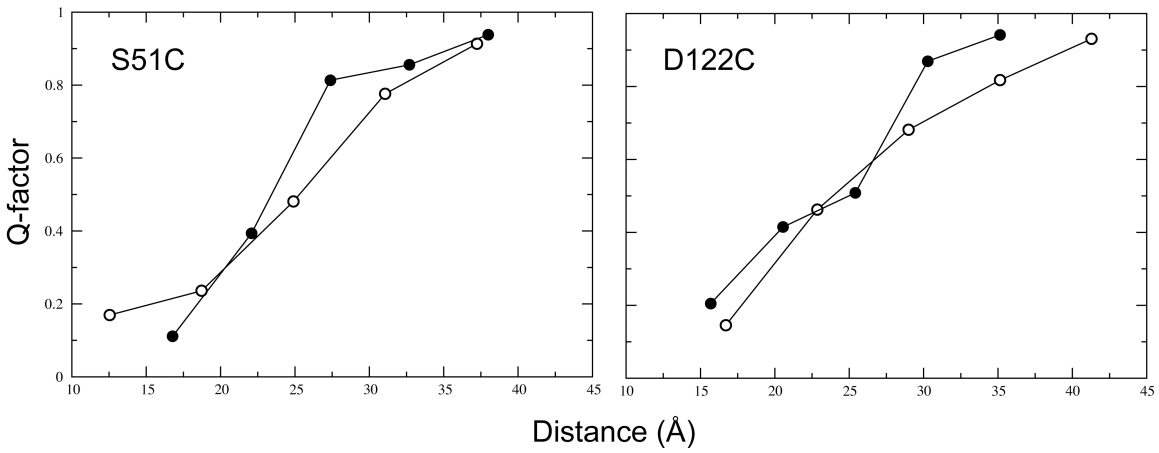

Figure S1. PRE Q-factor dependence on the effective paramagnet–$^{1}H^{N}$ distance. The effective distance between a nucleus and the paramagnetic center is defined by $(\langle r^{-6} \rangle)^{-1/6}$, where angular brackets indicate ensemble average over the three conformers used to represent the paramagnetic probe side chain. For each mutant and ligand state, such probe conformers were optimized against the associated experimental PRE data set and the corresponding crystal structure, as detailed in the Article. The 10 lowest-PRE energy optimizations were used to obtain average calculated PREs and average effective paramagnet–$^{1}H^{N}$ distances. The former were binned according to their associated distances (five bins in total, evenly dividing the distance range) and the Q-factor computed for each bin (excluding residues 143–149, 168, 169, and 173; see Article for details). The plots resulting from the S51C and D122C mutants are shown on the left and right panel, respectively. Open and full circles represent unliganded and liganded data sets, respectively.

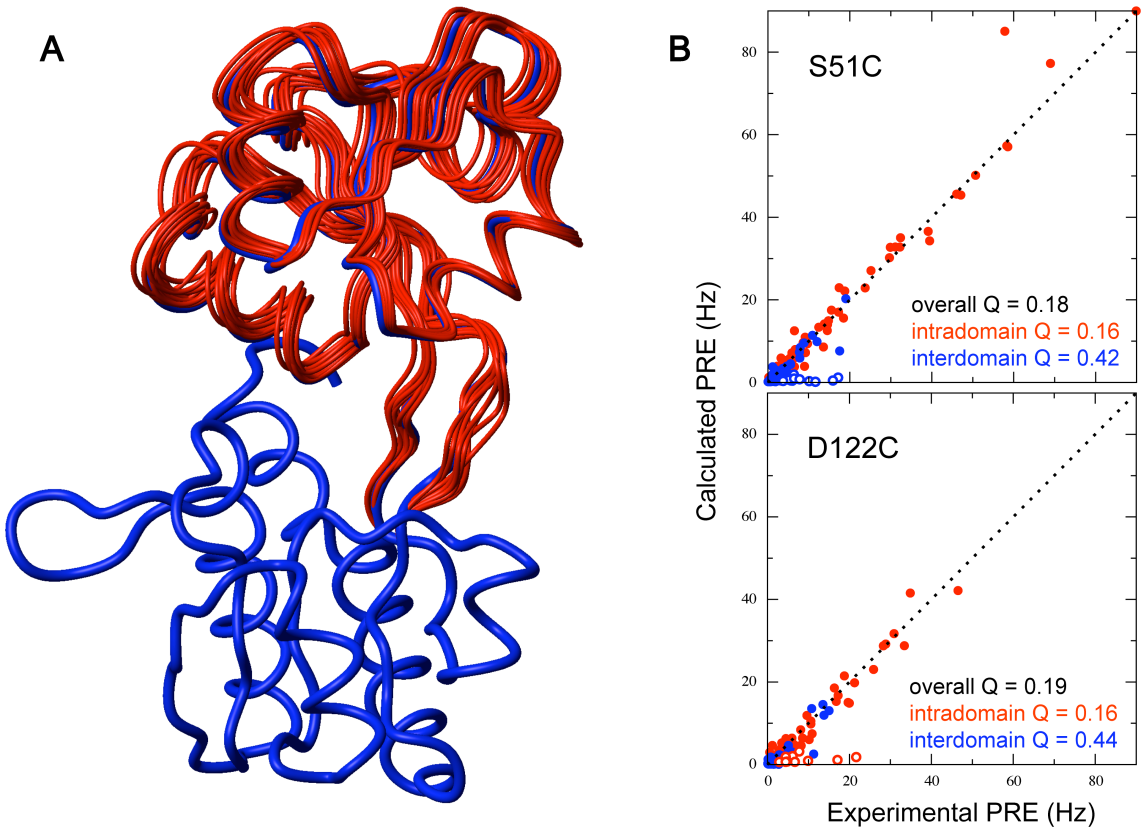

Figure S2. Refinement of the open ligand-free crystal structure of GlnBP (PDB ID 1GGG) against the S51C and D122C unliganded PRE data sets. The resulting structures are shown in panel A (red; 10 lowest-PRE energy models out of 200), superimposed to the crystal reference (blue) via the large domain. The associated correlation plots for the two data sets are displayed in panel B, where intradomain PREs are denoted by red circles, and interdomain by blue ones. The indicated Q-factors correspond to those of Table 2 in the Article. Open circles involve residues 143–149, 168, 169 and 173, and were used neither for refinement nor for Q-factor calculation (see Article for details).