Table S1. pK_a values of the charged residues on ferredoxin calculated by *H++*.

Residue Name	Complex 16			Complex 42		
	pK_a on Reduced Ferredoxin	pK_a on Oxidized Ferredoxin	ΔpK_a	pK_a on Reduced Ferredoxin	pK_a on Oxidized Ferredoxin	ΔpK_a
NTmet-1	7.810	7.797	0.013	7.343	7.324	0.019
TYR-3	13.025	12.992	0.033	12.931	12.907	0.024
LYS-4	11.158	11.150	0.008	11.212	11.202	0.010
LYS-8	11.835	11.803	0.032	12.454	12.431	0.023
ASP-13	1.833	1.815	0.018	1.320	1.303	0.017
LYS-14	10.733	10.719	0.014	10.308	10.281	0.027
GLU-17	4.217	4.211	0.006	4.304	4.296	0.008
CYS-18[1]	18.830	18.686	0.144	19.382	19.066	0.316
ASP-21	3.864	3.846	0.018	3.665	3.654	0.011
TYR-23[2]	14.230	14.005	0.225	14.696	14.203	0.493
ASP-26	1.831	1.393	0.438	2.831	2.195	0.636
GLU-29[3]	6.133	5.787	0.346	1.156	0.877	0.279
GLU-30	4.803	4.781	0.022	5.400	5.350	0.050
ASP-34	4.041	4.035	0.006	4.132	4.072	0.060
TYR-37[4]	13.751	13.483	0.268	15.135	14.770	0.365
ARG-40[5]	19.015	18.318	0.697	21.526	20.918	0.608
LYS-50	11.098	11.026	0.072	10.666	10.605	0.061
ASP-57	4.409	4.337	0.072	4.730	4.659	0.071
ASP-60	4.466	4.315	0.151	4.408	4.339	0.069
ASP-65	4.235	4.200	0.035	4.402	4.343	0.059
ASP-66	5.187	5.164	0.023	4.314	4.299	0.015
TYR-80[6]	20.355	20.237	0.118	13.095	13.132	-0.037
ASP-84	3.504	3.489	0.015	3.089	3.070	0.019
CYS-85[7]	17.860	17.572	0.288	16.336	16.076	0.260
HIP-90[8]	3.955	3.353	0.602	6.387	6.285	0.102
GLU-92	6.237	5.864	0.373	5.766	5.346	0.420
GLU-93	4.351	4.331	0.020	4.259	4.238	0.021
TYR-96	9.943	9.922	0.021	9.990	9.975	0.015
CTtyr-96	3.823	3.695	0.128	3.882	3.793	0.089

Notes:

1. Large pK_a due to the proximity to the carbonyl O atoms of PRO-19 and THR-22.
2. Large pK_a due to the proximity to the OH group of TYR-80.
3. The pK_a of complex 42 is smaller compared to that of complex 16 due to the closer distance to ARG-40 in complex 42.
4. Large pK_a due to the proximity to the GLU-29.
5. Large pK_a due to the proximity to ASP-26 and GLU-29.
6. The larger pK_a for complex 16 is caused by the closer distance to ASP-60 in complex 16.
7. Large pK_a due to the proximity to the carbonyl O atom of SER-83.
8. The pK_a of complex 16 is smaller than that of complex 42 because in complex 16 HIP-90 is buried inside protein, while in complex 42 it is on the surface.

Table S2. A sample APBS input file.

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end
elec
    mg-auto
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    cglen 200.0 200.0 200.0
    fglen 160.0 160.0 160.0
    cgcent mol 1
    fgcent mol 1
    mol 1
    sdens 40
    npbe
    bcfl mdh
    ion 1 0.050 2.0
    ion -1 0.050 2.0
    pdie 4.0
    sdie 78.5
    srfm smol
    chgm spl2
    srad 1.4
    swin 0.3
    temp 298.00
    gamma 0.105
    calcenergy total
    calcforce no
    write pot dx abc
end

quit
```

Figure S1. The spatial (A) and orientational occupancy landscapes (B) for $BD16_O$ at 50 mM ionic strength and a COM-COM distance of 36 Å. The color map in Fig. S1 –S5 is: blue-low and red-high.

A B

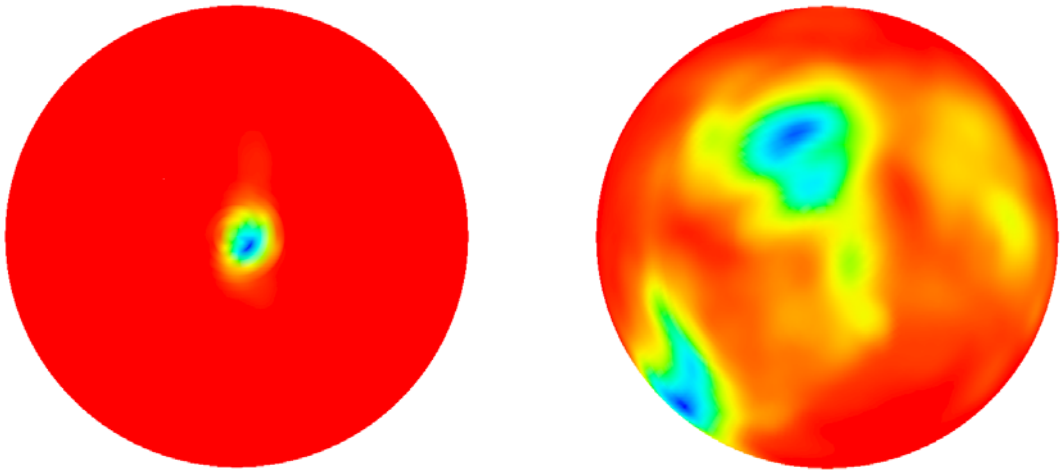

Figure S2. The spatial (A) and orientational occupancy landscapes (B) for $BD42_O$ at 50 mM ionic strength and a COM-COM distance of 40 Å.

A B

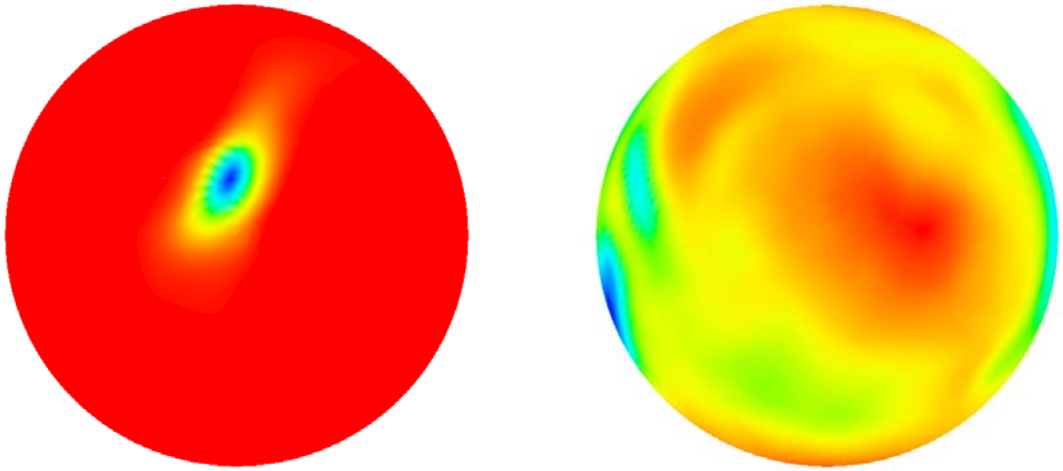

Figure S3. The configurations of $EC42B_R$ at 50 mM ionic strength (A) and at 150 mM ionic strength (B). The residue in purple is $Asp5_H$ and in green, $Glu93_F$.

A B

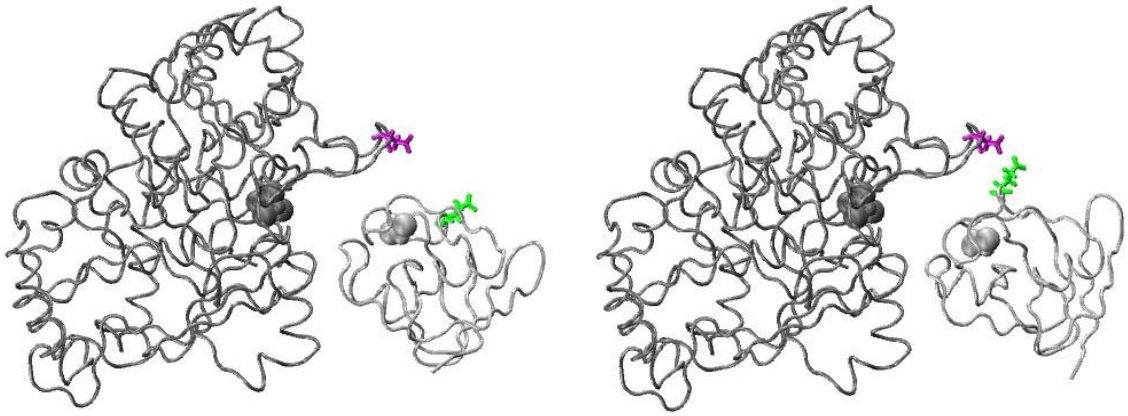

Figure S4. The free energy landscapes at 36 Å (A) and 40 Å (B) for $BD16_O$.

A B

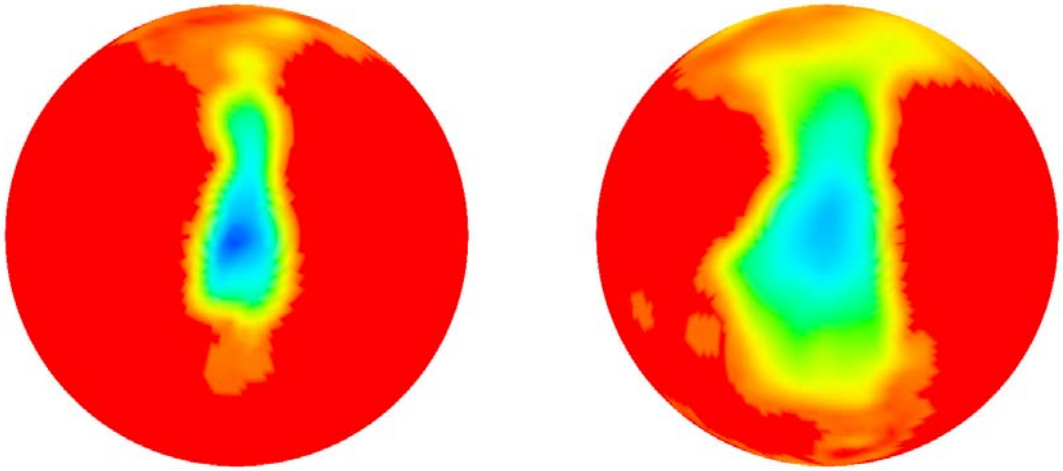

Figure S5. The free energy landscapes at 36 Å (A) and 40 Å (B) for $BD42_R$.

A B

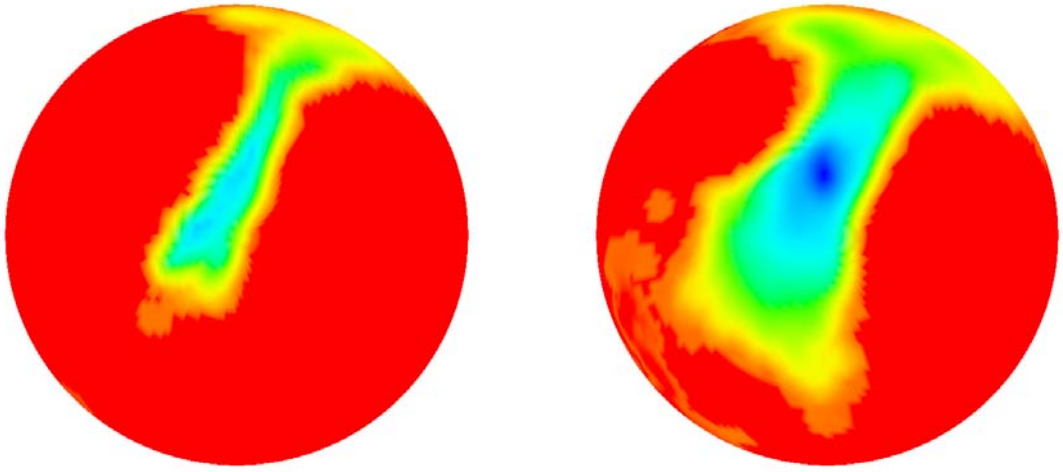

Figure S6. The free energy landscapes at 36 Å (A) and 40 Å (B) for $BD42_O$.

A B