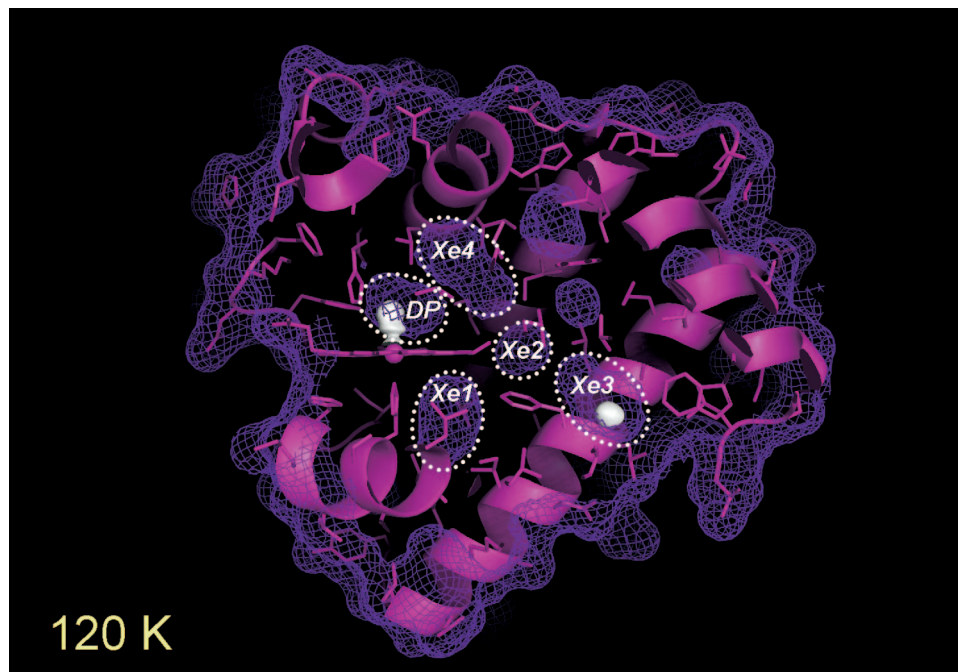


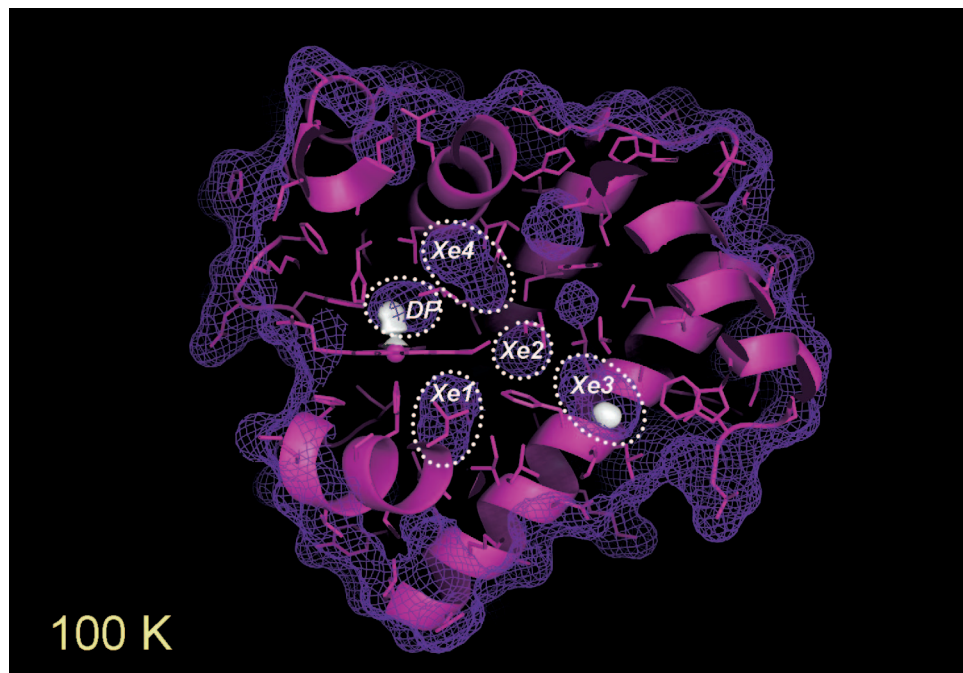
# Supporting Information

Tomita *et al.* 10.1073/pnas.0807774106



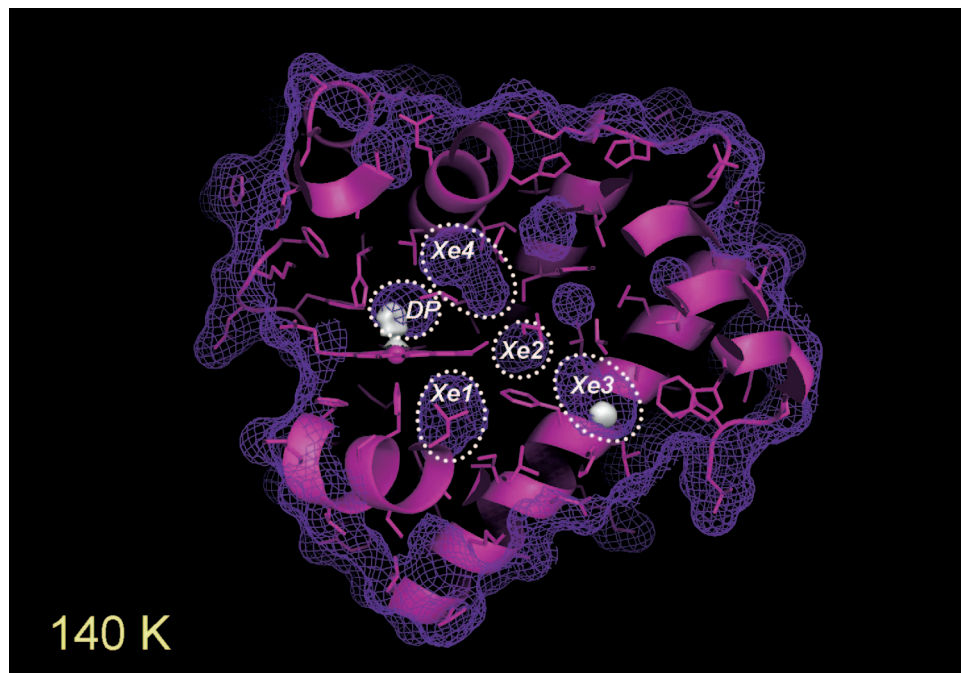
Movie S1. Ligand migration movie of MbCO at 120 K.

[Movie S1 \(AVI\)](#)



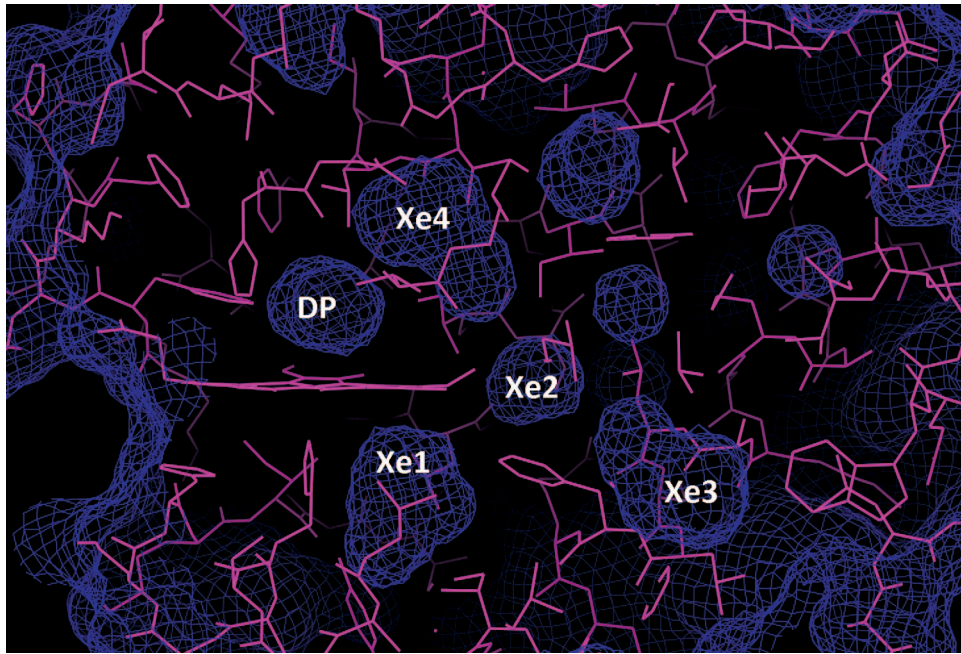
Movie S2. Ligand migration movie of MbCO at 100 K.

[Movie S2 \(AVI\)](#)



Movie S3. Ligand migration movie of MbCO at 140 K.

[Movie S3 \(AVI\)](#)



**Movie S4.** Movie of the tensor field of the structural changes represented by colored dots and 0.5-Å wires at 140 K.

[Movie S4 \(AVI\)](#)



**Table S2. The data collection and crystallographic analysis statistics at 120 K**

Statistic	Laser off	30 min	150 min	300 min	450 min	600 min	750 min	810 min
Space group	P 1 2 <sub>1</sub> 1	P 1 2 <sub>1</sub> 1	P 1 2 <sub>1</sub> 1	P 1 2 <sub>1</sub> 1	P 1 2 <sub>1</sub> 1	P 1 2 <sub>1</sub> 1	P 1 2 <sub>1</sub> 1	P 1 2 <sub>1</sub> 1
Cell dimensions a, Å	34.536	34.425	34.431	34.439	34.446	34.453	34.460	34.462
b, Å	30.847	30.720	30.723	30.724	30.721	30.718	30.715	30.714
c, Å	63.897	63.843	63.861	63.876	63.891	63.907	63.923	63.932
$\beta$ , °	105.647	105.541	105.542	105.553	105.570	105.588	105.607	105.617
Wavelength, Å	0.827	0.827	0.827	0.827	0.827	0.827	0.827	0.827
Resolution, Å	50.0–1.22	50.0–1.21	50.0–1.21	50.0–1.21	50.0–1.21	50.0–1.21	50.0–1.21	50.0–1.21
$R_{\text{merge}}$	0.039(0.469)	0.052(0.253)	0.056(0.275)	0.051(0.310)	0.049(0.354)	0.053(0.380)	0.055(0.406)	0.054(0.421)
$I/\sigma$	9.5(1.1)	13.2(2.4)	12.9(2.2)	12.4(1.9)	11.7(1.7)	11.1(1.5)	10.7(1.4)	10.6(1.3)
Completeness	0.835(0.377)	0.981(0.874)	0.979(0.829)	0.979(0.803)	0.982(0.782)	0.972(0.706)	0.959(0.645)	0.952(0.586)
Redundancy	3.2(2.0)	3.6(2.9)	3.6(2.9)	3.6(2.8)	3.6(2.6)	3.6(2.3)	3.5(2.1)	3.5(2.0)
No. reflections	33,220	38,789	38,772	38,802	38,766	38,508	38,082	37,777
$R$ factor	0.153	0.143	0.142	0.141	0.142	0.144	0.145	0.146
$R_{\text{free}}$	0.207	0.182	0.182	0.179	0.183	0.186	0.188	0.191
No. atoms	1,438	1,442	1,443	1,441	1,441	1,435	1,433	1,429
Mean $B$ value	15.257	14.612	14.799	14.814	15.029	15.052	15.149	15.139
rmsd bond length, Å	0.027	0.018	0.018	0.019	0.020	0.020	0.022	0.022
rmsd angle, °	2.179	1.787	1.877	1.867	1.863	1.908	1.980	2.015

Values in parentheses are for the highest-resolution shell (1.25–1.21 Å).

