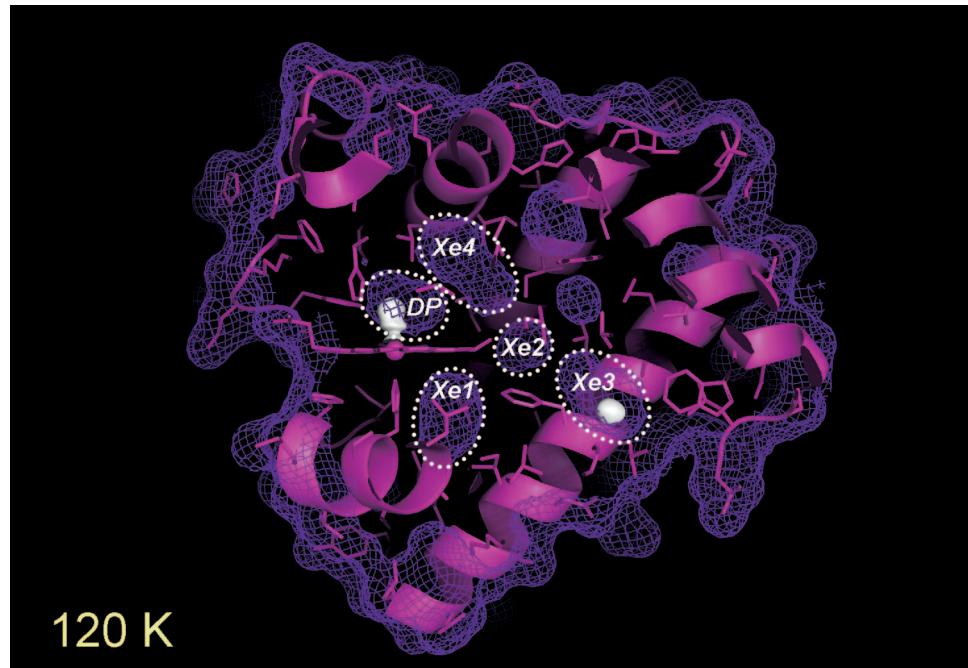


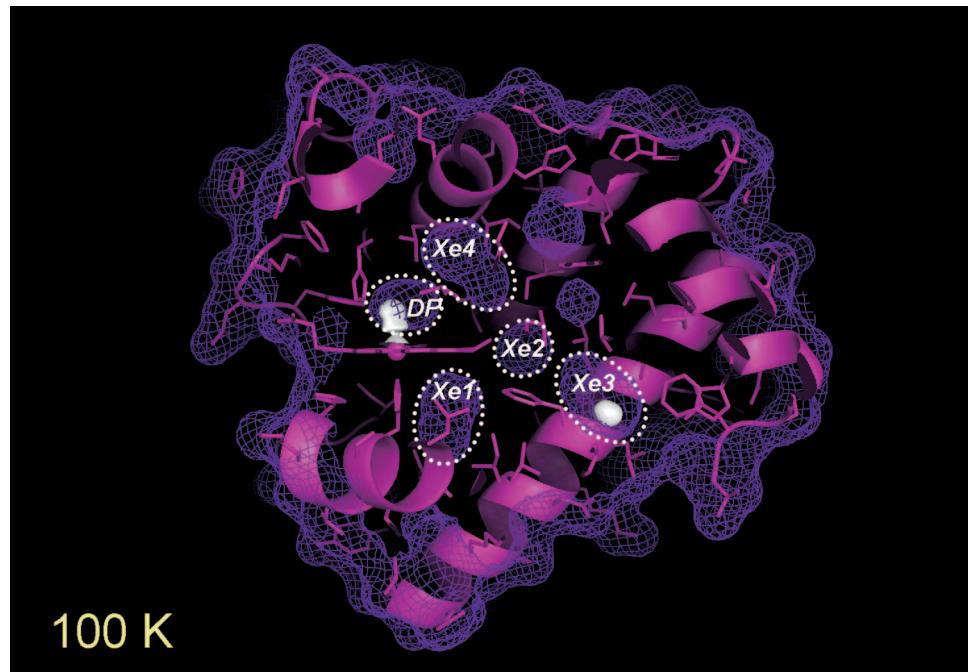
Supporting Information

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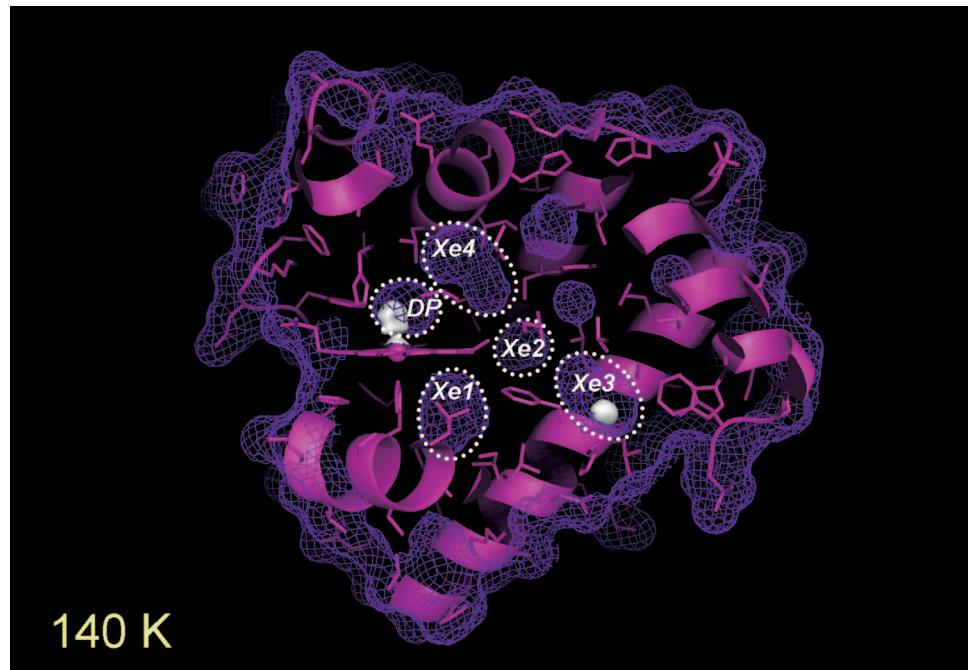
Movie S1. Ligand migration movie of MbCO at 120 K.

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



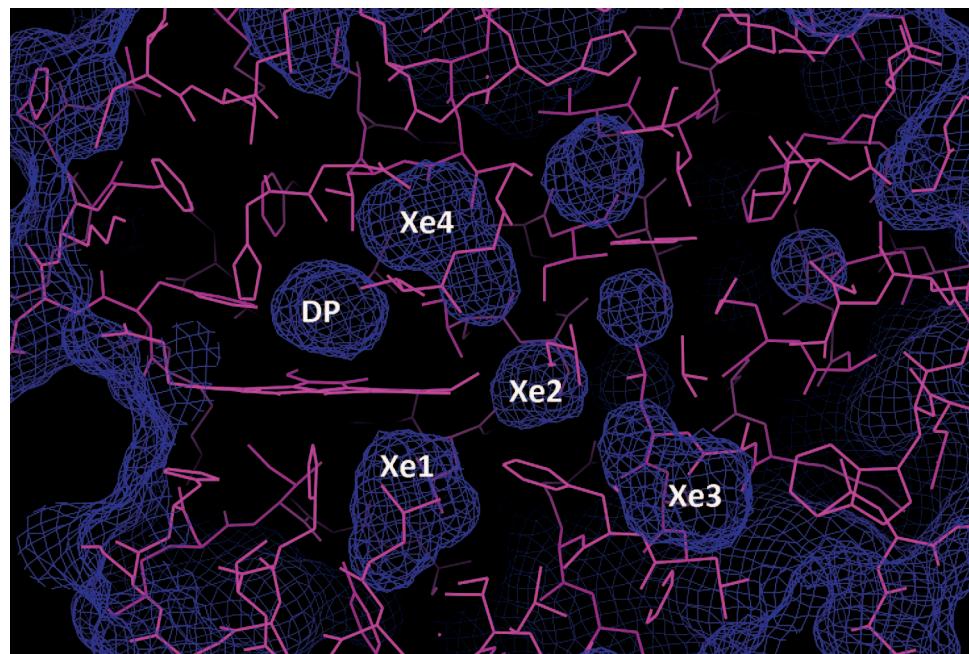
Movie S2. Ligand migration movie of MbCO at 100 K.

[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 S1. The data collection and crystallographic analysis statistics at 100 K

Statistic	Laser off	30 min	150 min	300 min	450 min	600 min	750 min	810 min
Space group	P 1 2 ₁ 1							
Cell dimensions a, Å	34.319	34.325	34.329	34.333	34.342	34.350	34.377	34.383
b, Å	30.604	30.612	30.625	30.631	30.635	30.633	30.611	30.615
c, Å	63.618	63.634	63.664	63.693	63.714	63.729	63.750	63.761
β , °	105.388	105.381	105.358	105.349	105.356	105.366	105.452	105.454
Wavelength, Å	0.827	0.827	0.827	0.827	0.827	0.827	0.827	0.827
Resolution, Å	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	50.0–1.21
R_{merge}	0.047(0.361)	0.047(0.372)	0.046(0.390)	0.050(0.426)	0.052(0.405)	0.052(0.429)	0.048(0.492)	0.050(0.530)
$\text{I}/\sigma_{\text{I}}$	11.7(1.6)	11.5(1.5)	11.2(1.4)	10.8(1.3)	10.4(1.3)	10.1(1.2)	10.3(1.1)	10.1(0.9)
Completeness	0.952(0.713)	0.950(0.638)	0.932(0.576)	0.907(0.480)	0.884(0.392)	0.857(0.267)	0.816(0.202)	0.827(0.221)
Redundancy	3.6(2.6)	3.6(2.5)	3.6(2.4)	3.6(2.3)	3.5(2.0)	3.5(1.8)	3.5(1.9)	3.5(1.8)
No. reflections	35,237	35,188	34,877	33,991	33,200	32,183	30,673	30,794
R factor	0.153	0.155	0.153	0.154	0.152	0.153	0.152	0.152
R_{free}	0.205	0.211	0.211	0.209	0.212	0.210	0.219	0.222
No. atoms	1,446	1,445	1,444	1,440	1,433	1,433	1,421	1,421
Mean B value	15.523	15.538	15.541	15.756	15.656	15.758	15.658	15.759
rmsd bond length, Å	0.023	0.023	0.023	0.024	0.024	0.025	0.025	0.027
rmsd angle, °	1.962	2.070	2.063	2.113	2.208	2.229	2.201	2.326

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

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 ₁ 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
β , °	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_{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)
$\text{I}/\sigma_{\text{sigma}}$	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_{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).

Table S3. The data collection and crystallographic analysis statistics at 140 K

Statistic	Laser off	30 min	150 min	300 min	450 min	600 min	750 min
Space group	P 1 2_1 1						
Cell dimensions a, Å	34.343	34.347	34.353	34.371	34.373	34.377	34.381
b, Å	30.613	30.620	30.621	30.614	30.592	30.571	30.549
c, Å	63.785	63.799	63.805	63.809	63.814	63.825	63.841
β , °	105.865	105.866	105.845	105.788	105.730	105.680	105.629
Wavelength, Å	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
R_{merge}	0.052(0.465)	0.053(0.535)	0.051(0.491)	0.053(0.638)	0.054(0.775)	0.056(0.478)	0.056(0.127)
$\text{I}/\sigma_{\text{I}}$	8.6(1.1)	8.6(0.9)	8.8(0.9)	8.5(0.7)	8.0(0.4)	7.8(0.4)	7.5(0.2)
Completeness	0.894(0.341)	0.889(0.383)	0.892(0.374)	0.835(0.269)	0.805(0.211)	0.758(0.147)	0.721(0.176)
Redundancy	3.4(1.6)	3.4(1.6)	3.3(1.5)	3.3(1.4)	3.2(1.3)	3.1(1.2)	3.0(1.3)
No. reflections	35,428	35,228	35,374	33,117	31,909	30,123	28,702
R factor	0.156	0.167	0.165	0.158	0.163	0.168	0.169
R_{free}	0.209	0.220	0.219	0.217	0.226	0.240	0.240
No. atoms	1,437	1,431	1,430	1,421	1,416	1,411	1,402
Mean B value	15.918	16.648	16.812	16.238	16.817	17.307	17.409
rmsd bond length, Å	0.029	0.035	0.034	0.032	0.036	0.041	0.046
rmsd angle, °	2.394	2.971	2.982	2.661	2.936	3.247	3.377

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