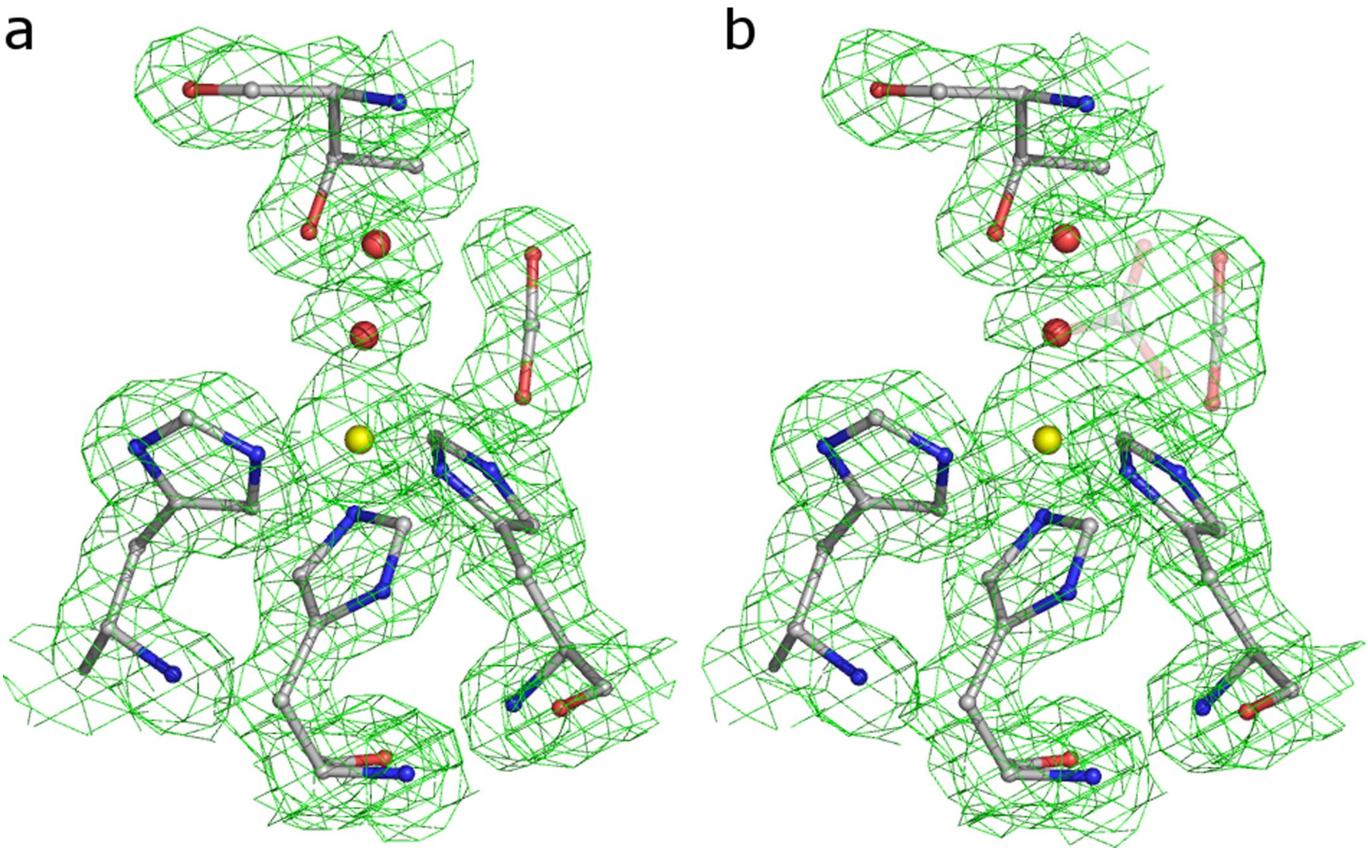
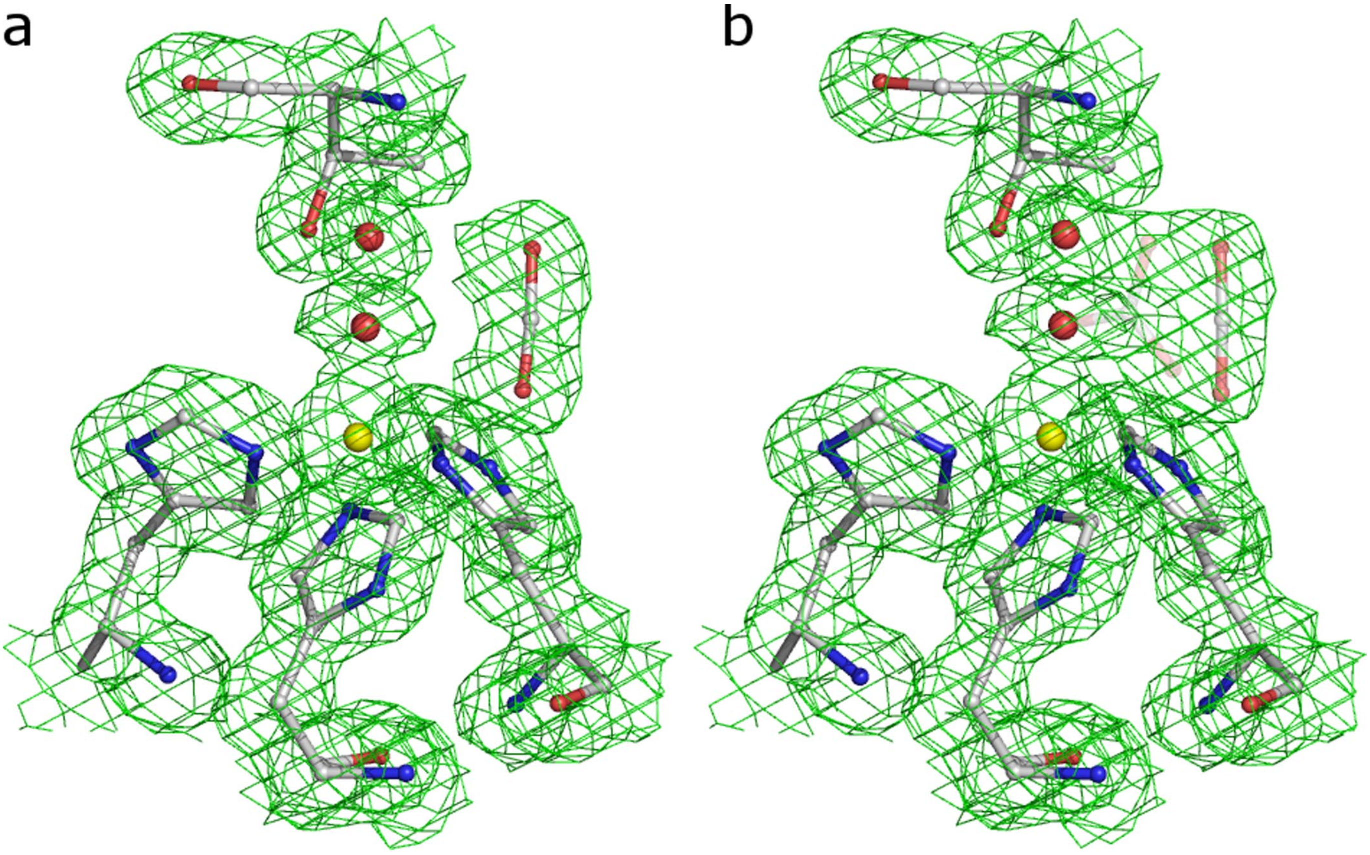
Supporting Information

Sjöblom et al. 10.1073/pnas.0904184106



Movie S1. Substrate-to-product conversion in the active site of HCAII using diffraction data collected at 1.278-Å wavelength. Shown above are the first (*a*) and last (*b*) images of the movie. The movie presents 103 refined models together with the final $2|F_o| - |F_c|$ map contoured at 1σ level. The movie starts in a state corresponding to the HCAII:CO_2 complex, proceeds through decreasing substrate to product ratios, and ends in a state with 65% CO_2 and 35% HCO_3^- at delivered dose corresponding to 30% Henderson limit. The occupancy of carbon dioxide and bicarbonate is represented by the transparency of the models.

Movie S1 (GIF)



Movie S2. Substrate to product conversion in the active site of HCAII using diffraction data collected at 0.94-Å wavelength. Shown above are the first (*a*) and last (*b*) images of the movie. The movie presents 11 refined models together with the final $2|F_o| - |F_c|$ map contoured at 1σ level. The movie starts in a state corresponding to the HCAII:CO_2 complex, proceeds through decreasing substrate to product ratios, and ends in a state with 70% CO_2 and 30% HCO_3^- at delivered dose corresponding to 30% Henderson limit. The occupancy of carbon dioxide and bicarbonate is represented by the transparency of the models.

Movie S2 (GIF)

Table S1. First movie data collection and refinement statistics

	First set	Last set
Data collection		
Beamline	X11, EMBL/DESY	X11, EMBL/DESY
Wavelength, Å	1.278	1.278
Flux, photons per second*	3.6×10^{10}	
Space group	$P2_1$	$P2_1$
Cell	$a = 42.17$ Å, $b = 41.45$ Å, $c = 72.36$ Å, $\beta = 103.9°$	$a = 42.17$ Å, $b = 41.45$ Å, $c = 72.36$ Å, $\beta = 103.9°$
Unique reflections	28,729	28,824
Resolution, Å	19.88–1.66 (1.75–1.66)	19.88–1.66 (1.75–1.66)
Redundancy	3.7 (3.4)	3.7 (3.4)
Completeness, %	99.2 (95.1)	99.3 (95.5)
R_{merge}	0.036 (0.142)	0.035 (0.156)
Refinement		
No. of reflections	27,250	27,341
R value	0.176	0.176
R_{free}	0.222	0.219
rmsd from ideality, bonds, Å	0.017	0.014
rmsd from ideality, angles, °	1.721	1.563
Overall B, Å^2	17.0	17.6

Numbers in parentheses refer to the last resolution shell. $R_{\text{merge}} = \Sigma|I_i - \langle I\rangle|/\Sigma I_i$, where I_i is the intensity of an individual reflection and $\langle I\rangle$ is the mean intensity of that reflection. R value $= \Sigma|F_o - F_c|/\Sigma F_o$. R_{free} is the cross-validation R value computed for a subset of reflections, omitted in the refinement process (5% of the total number of reflections).

*Data were collected in dose mode.

Table S2. Second movie data collection and refinement statistics

	First set	Last set
Data collection		
Beamline	ID14-4, ESRF	ID14-4, ESRF
Wavelength, Å	0.94	0.94
Flux, photons per second	7.2×10^{11}	6.9×10^{11}
Space group	$P2_1$	$P2_1$
Cell	$a = 42.20$ Å, $b = 41.49$ Å, $c = 72.39$ Å, $\beta = 104.0°$	$a = 42.20$ Å, $b = 41.49$ Å, $c = 72.39$ Å, $\beta = 104.0°$
Unique reflections	38,406	38,993
Resolution, Å	41.49–1.50 (1.58–1.50)	41.49–1.50 (1.58–1.50)
Redundancy	3.6 (3.6)	3.6 (3.6)
Completeness, %	98.3 (99.2)	98.9 (98.7)
R_{merge}	0.056 (0.127)	0.061 (0.275)
Refinement		
No. of reflections	36,425	36,964
R value	0.193	0.189
R_{free}	0.242	0.233
rmsd from ideality, bonds, Å	0.017	0.017
rmsd from ideality, angles, °	1.731	1.742
Overall B, Å^2	18.8	19.7

Numbers in parentheses refer to the last resolution shell. $R_{\text{merge}} = \Sigma|I_i - \langle I\rangle|/\Sigma I_i$, where I_i is the intensity of an individual reflection and $\langle I\rangle$ is the mean intensity of that reflection. R value $= \Sigma|F_o - F_c|/\Sigma F_o$. R_{free} is the cross-validation R value computed for a subset of reflections, omitted in the refinement process (5% of the total number of reflections).