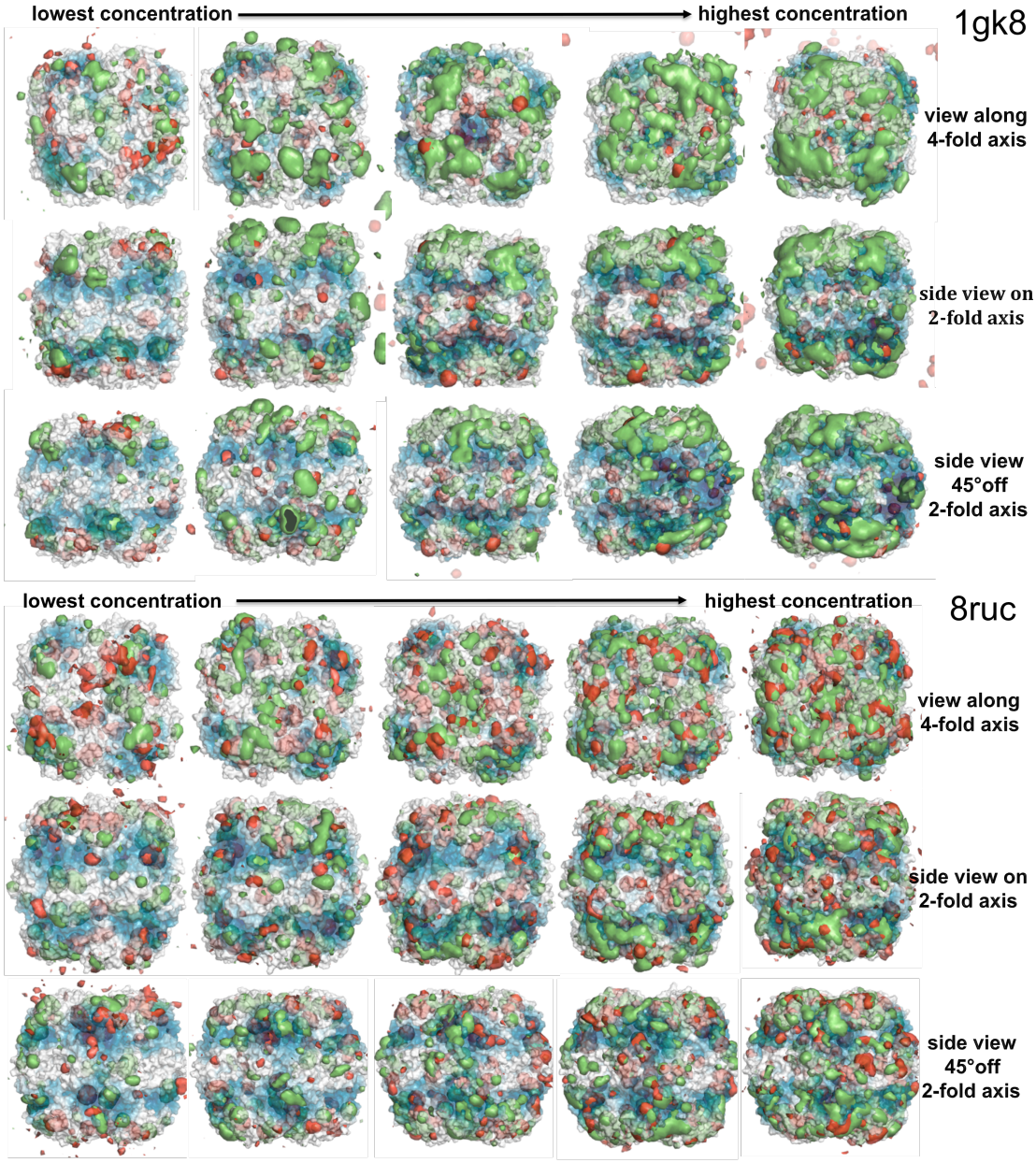
CO_2 and O_2 Distribution in Rubisco Suggests the Small Subunit Functions as a CO_2 Reservoir

Michiel van Lun,[†] Jochen S. Hub,[‡,§] David van der Spoel[‡] and Inger Andersson[‡,*]

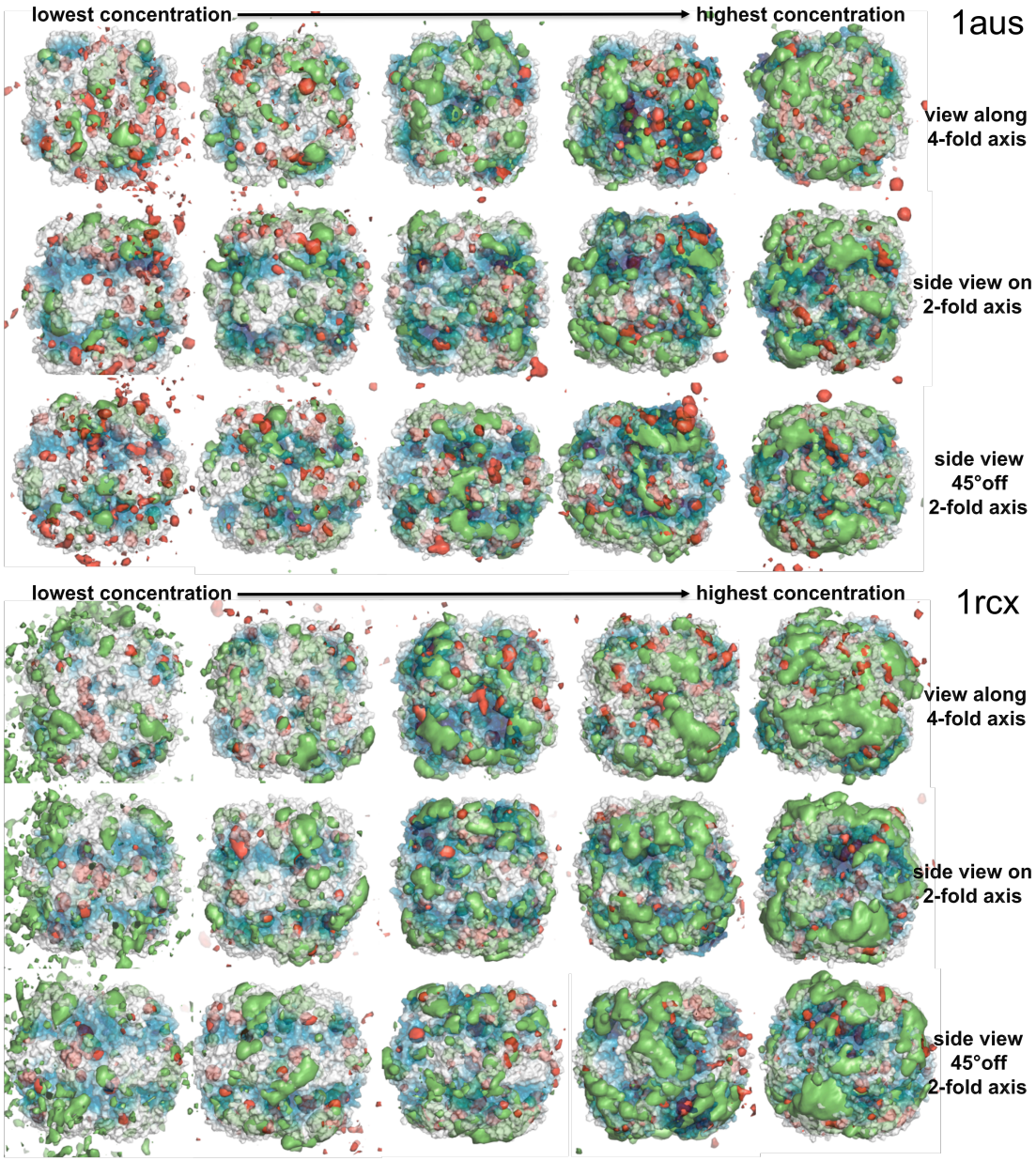
[†]*Department of Molecular Biology, Swedish University of Agricultural Sciences, Box 590, S-751 24 Uppsala, Sweden.* [‡]*Department of Cell and Molecular Biology, Uppsala University, Box 596, S-751 24 Uppsala Sweden.* [§]*Georg-August-University Göttingen, Institute for Microbiology and Genetics, Justus-von-Liebig-Weg 11, 37077 Göttingen, Germany.*

Supporting information

Supporting Figure 1. Density maps of CO_2 and O_2 in Rubisco and surrounding solvent. The protein surface is shown as a gradient of white to blue, with darkest blue indicating the center of the active sites. The protein surface is transparent to show the inside location of CO_2 and O_2 (green and red, respectively, 2 sigma cutoff). From left to right are snapshots from simulations with increasing amount of CO_2 or O_2 for four Rubisco structures from *C. reinhardtii* (PDB code 1gk8) and spinach (PDB codes 8ruc, 1aus, 1rcx). Three views are shown for each concentration.



Supporting Figure 1 ctd.



Supporting Figure 2. Total number of CO_2 (upper panel) and O_2 (lower panel) molecules per residue, on a logarithmic scale, from simulations at the highest (C)O_2 concentration. The complexes are denoted by their PDB code, see Methods Section for details. The number of contacts per residue is calculated cumulatively and per available solvent accessible surface area of each residue.