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Supporting information for article:

Unravelling the shape and structural assembly of photosynthetic GAPDH–CP12–PRK complex from *Arabidopsis thaliana* by small-angle X-ray scattering analysis

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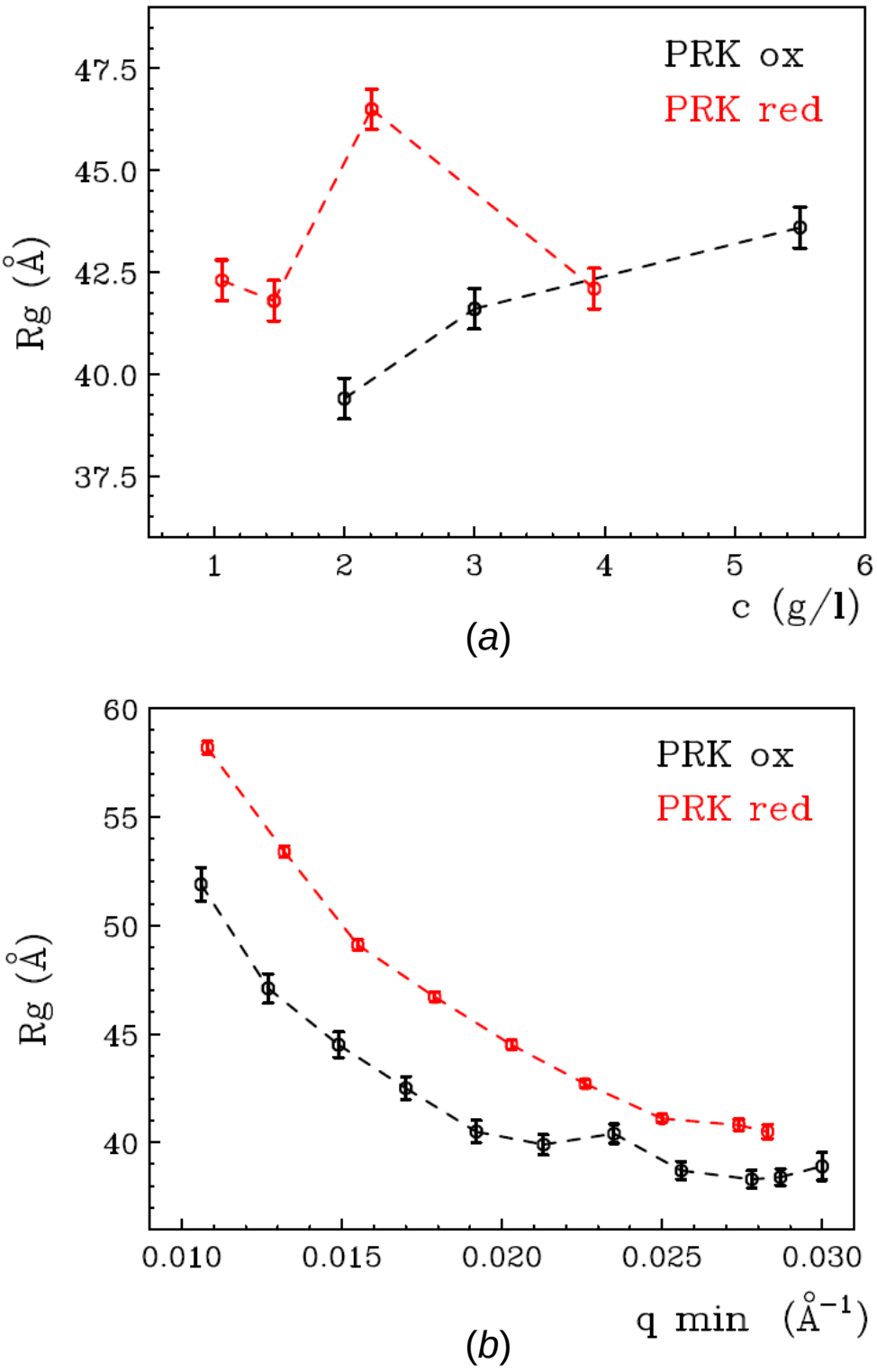

Figure S1

Giration radius (R_g) distributions for oxidized and reduced PRK.(*a*) R_g values obtained from the Guinier linear fit for oxidized (black) and reduced (red) PRK at increasing concentrations. (*b*) R_g values obtained from the Guinier linear fit for oxidized (2.0 mg·ml^{-1}) and reduced (3.92 mg·ml^{-1}) PRK experimental data considering different q-intervals, at increasing values of the minimum scattering vector (q_{min}) included.

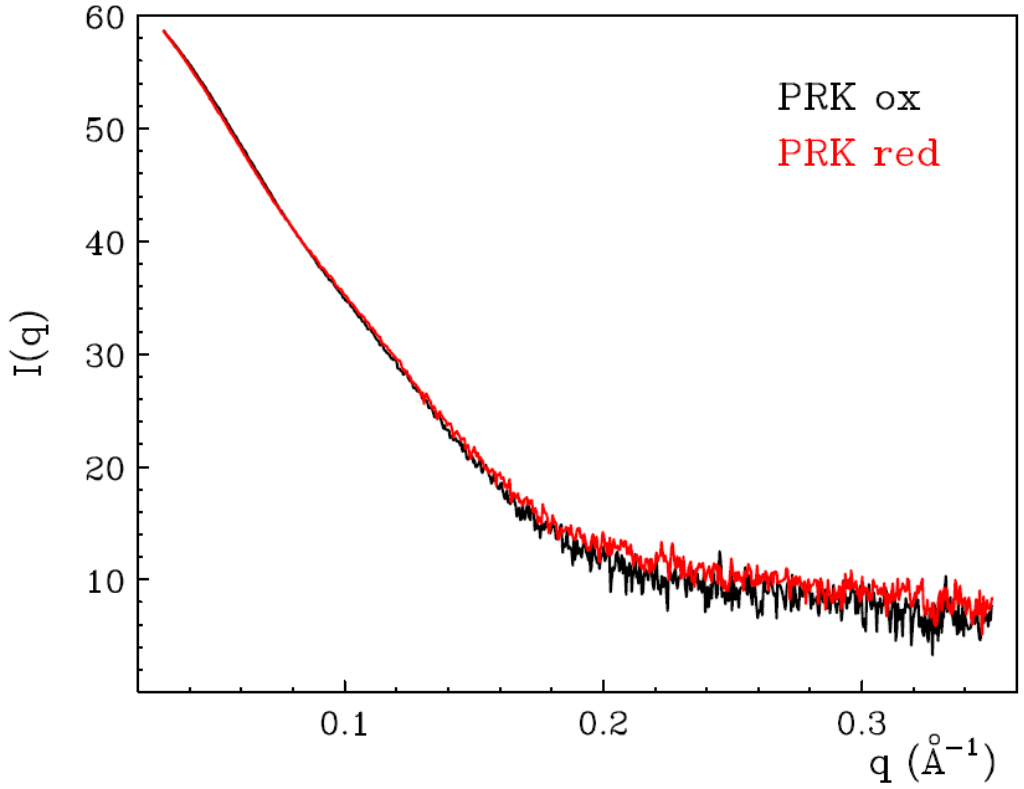

Figure S2
Superimposition of the SAXS experimental curves (log scale) obtained from oxidized (black) and reduced (red) PRK.

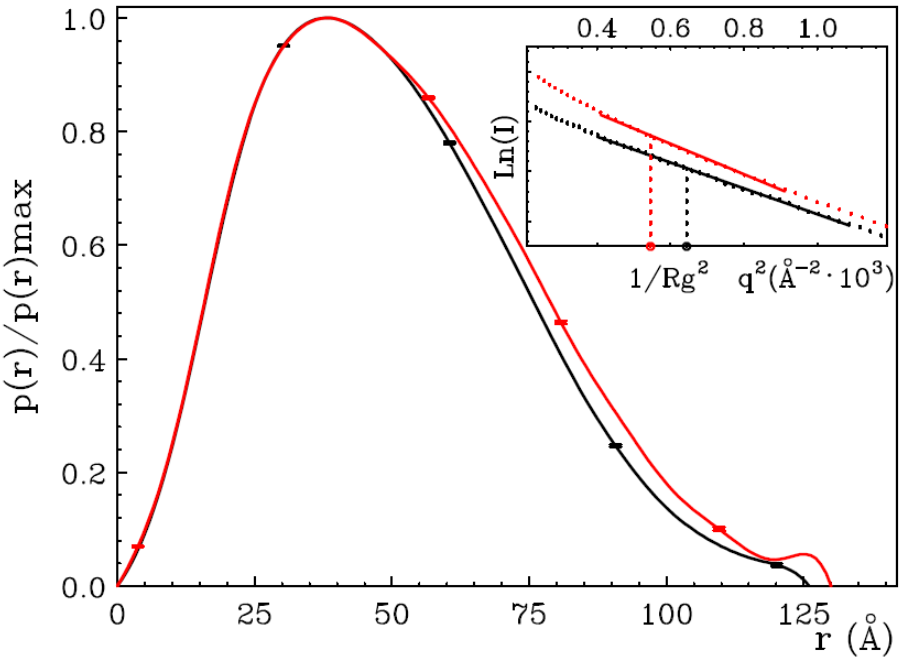

Figure S3
p(r) functions for oxidized (black) and reduced (red) PRK normalized for their maximum value. Only few error bars are shown for the sake of clarity. In the inset the Guinier plot (dots) and the linear fit are shown for oxidized (black) and reduced (red) PRK.

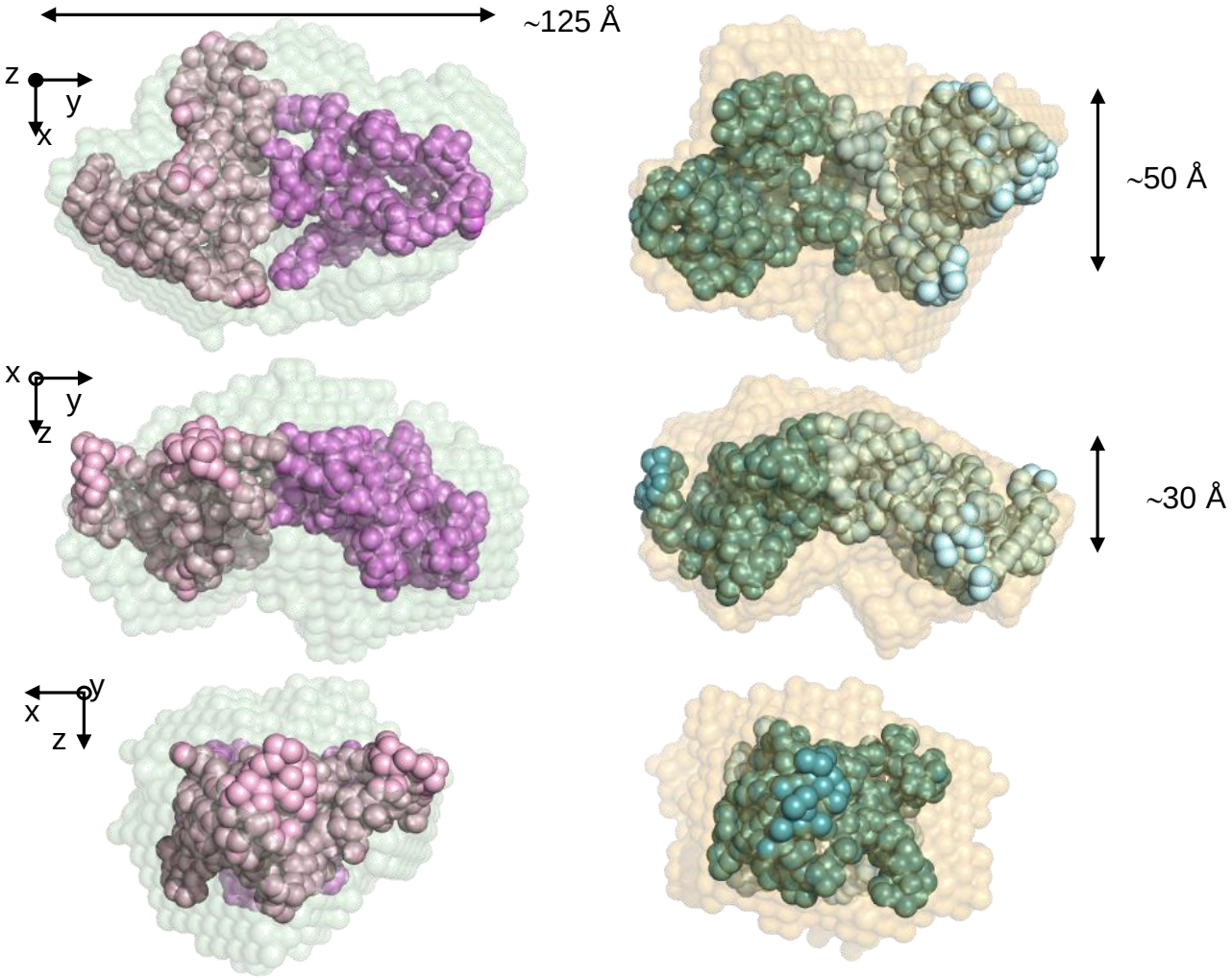

Figure S4
Dummy residues models for oxidized PRK computed by GASBOR with P1 (left) and P2 (right) symmetry. The models are superimposed to the overall probability maps coming from the superimposition of 20 models compared using DAMCLUST, and include all the positions occupied by the dummy residues of models belonging to the same most representative cluster. Not all of these positions have the same occupancy probability.

Table S1. Normalized spatial discrepancy (NSD) values for the ab-initio models of oxidized PRK computed by GASBOR with P2 or P1 symmetry.

GASBOR models	<NSD> (all)	N. models in main cluster	<NSD> (main cluster)
P2	1.691±0.038	10	1.690
P1	1.706±0.039	10	1.607

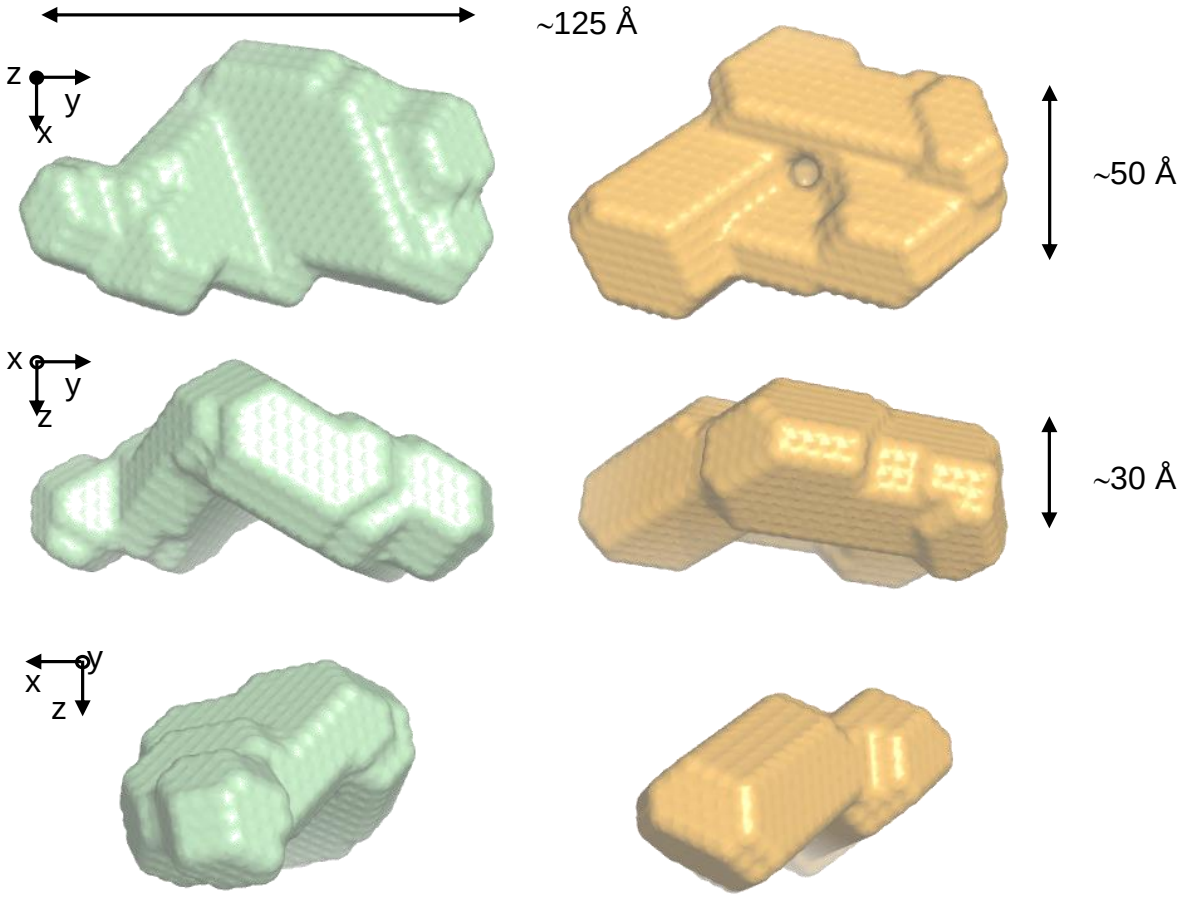

Figure S5.
Dummy atoms models computed by DAMMIF with P1 symmetry for reduced PRK (left) and oxidized PRK (right).

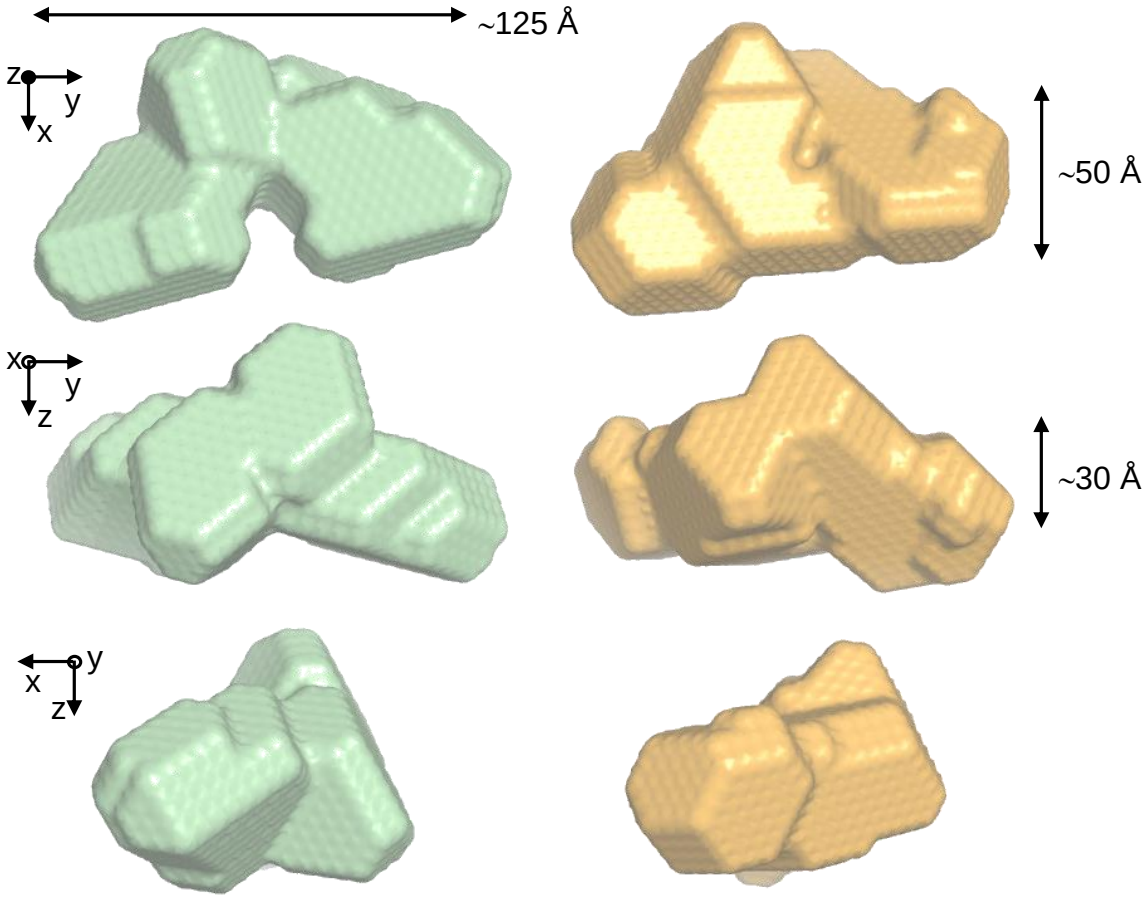

Figure S6.
Dummy atoms models computed by DAMMIF with P2 symmetry for reduced PRK (left) and oxidized PRK (right).

Table S2. Normalized spatial discrepancy (NSD) values for the ab-initio models of oxidized and reduced PRK computed by DAMMIF with P2 or P1 symmetry.

DAMMIF models		<NSD> (all)	<NSD> (main cluster)
P2	Ox. PRK	1.503±0.262	0.933
	Red. PRK	1.567±0.304	0.995
P1	Ox. PRK	0.830±0.035	0.777
	Red. PRK	0.821±0.048	0.733

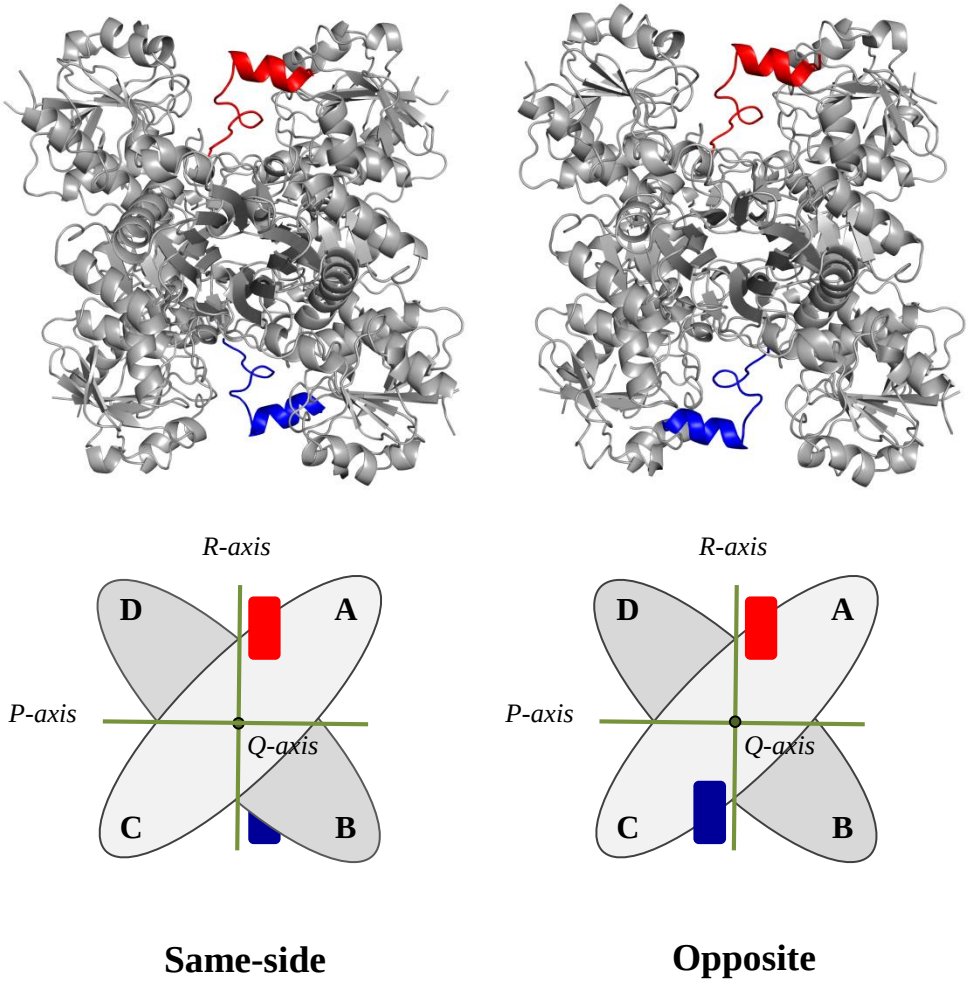

Figure S7

The binding of CP12 to the GADPH tetramer in "same-side" and "opposite" conformations of GADPH/CP12 complex from the crystallographic structure (PDB code 2QV1; Fermani et al., 2012), is shown as cartoon (upper panel) and as a schematic (lower panel) representation. The GADPH chains are labeled accordingly to the structure and the molecular symmetry axes are indicated. In the "same-side" conformation the two CP12s are identically oriented with respect to the R-axis; one CP12 (red) occupies the position in front of GAPDH chain A and the second CP12 (blue) occupies the position behind GAPDH chain B. In the "opposite" conformation the two CP12s are oriented in the opposite way with respect to the R-axis; both CP12s occupy the position in front of GAPDH chains A and C.

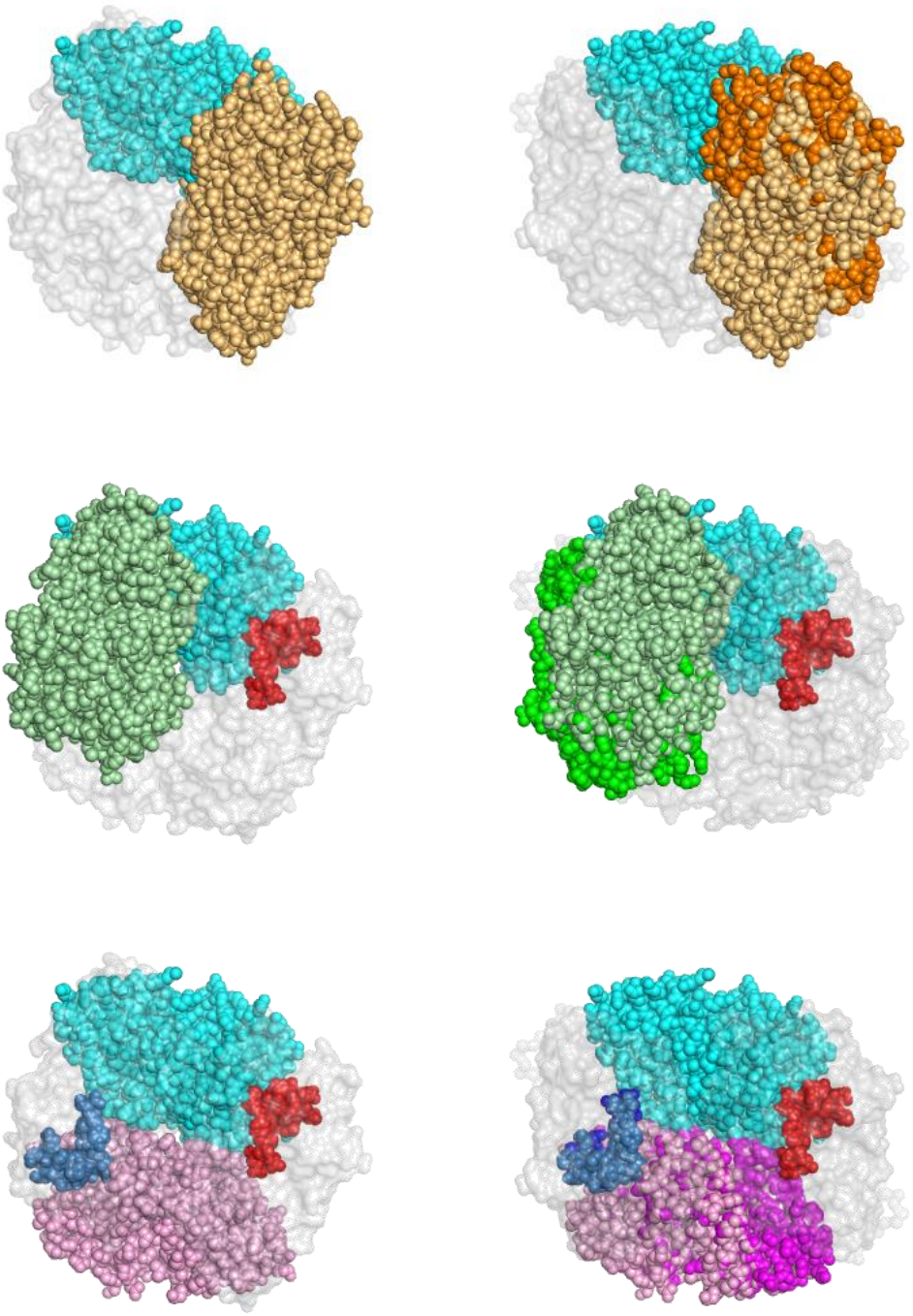

Figure S8
Superimposition between the crystallographic structure and the rigid-body optimized model of the GAPDH/CP12 complex. On the left, the crystal structure (PDB code 2QV1; Fermani et al., 2012) is shown. On the right, the rigid-body optimized subunits are superimposed to the crystallographic ones in brighter colors, assuming subunit A as reference. The GAPDH subunits are highlighted in couples for clarity, from the top: A and B, A and C, A and D. The six chains are represented as sphere in different colors (chain A cyan, B magenta, C green, D orange, G(CP12) red, H(CP12) blue).

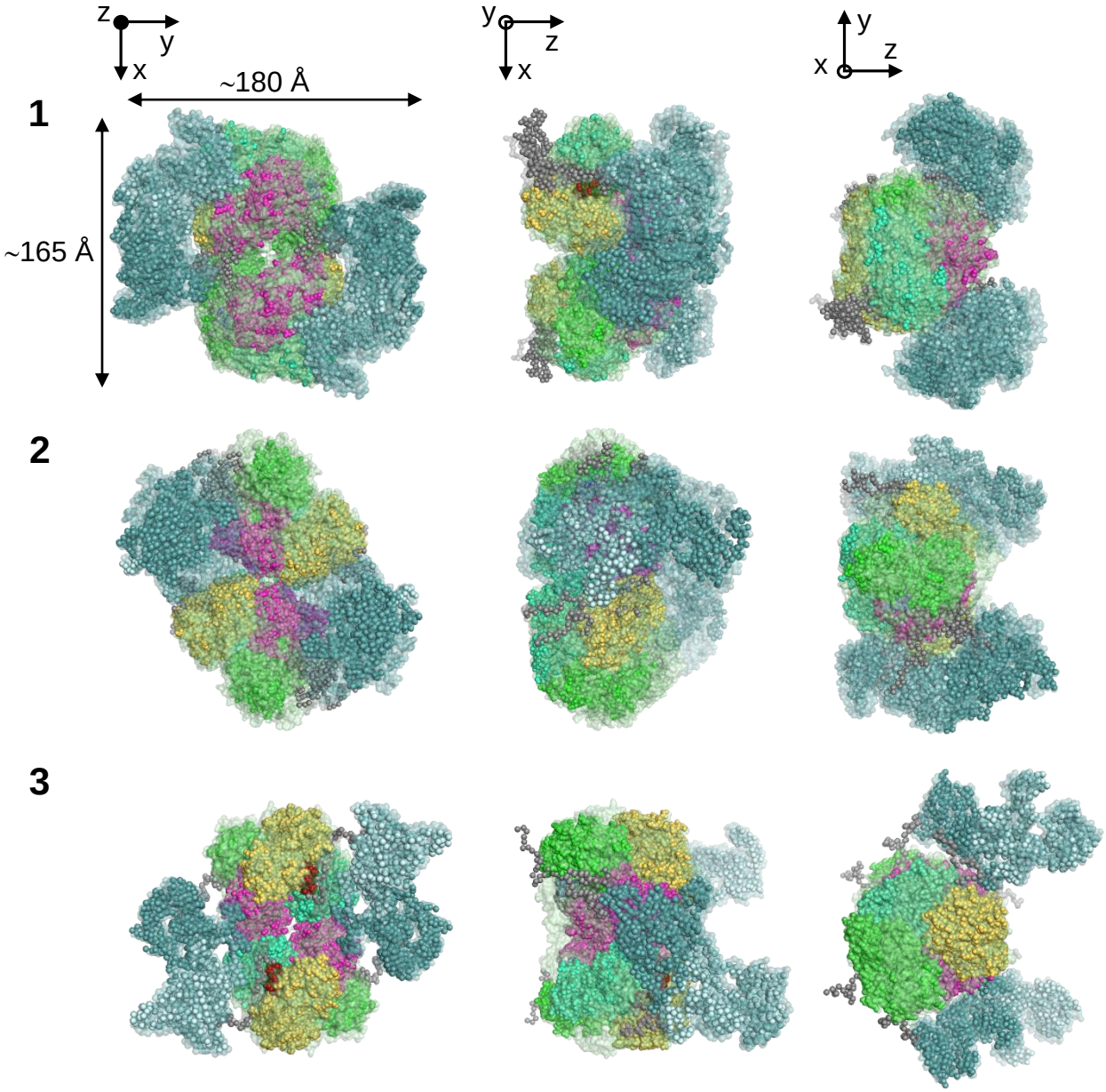

Figure S9
Superposition of GAPDH/CP12/PRK complex rigid-body optimized models. The models belonging to the each assembly named 1 or 2 or 3, have been superimposed. In the reference models, GAPDH tetramers (chain A in cyan, B in magenta, C in green and D in orange), PRK dimers (monomers in cyan and deep cyan) and CP12s (chain G in red, H in blue and the N-terminal dummy residues in gray) are represented as spheres. The superimposed models are rendered as transparent surfaces. Three orthogonal orientations are visualized.

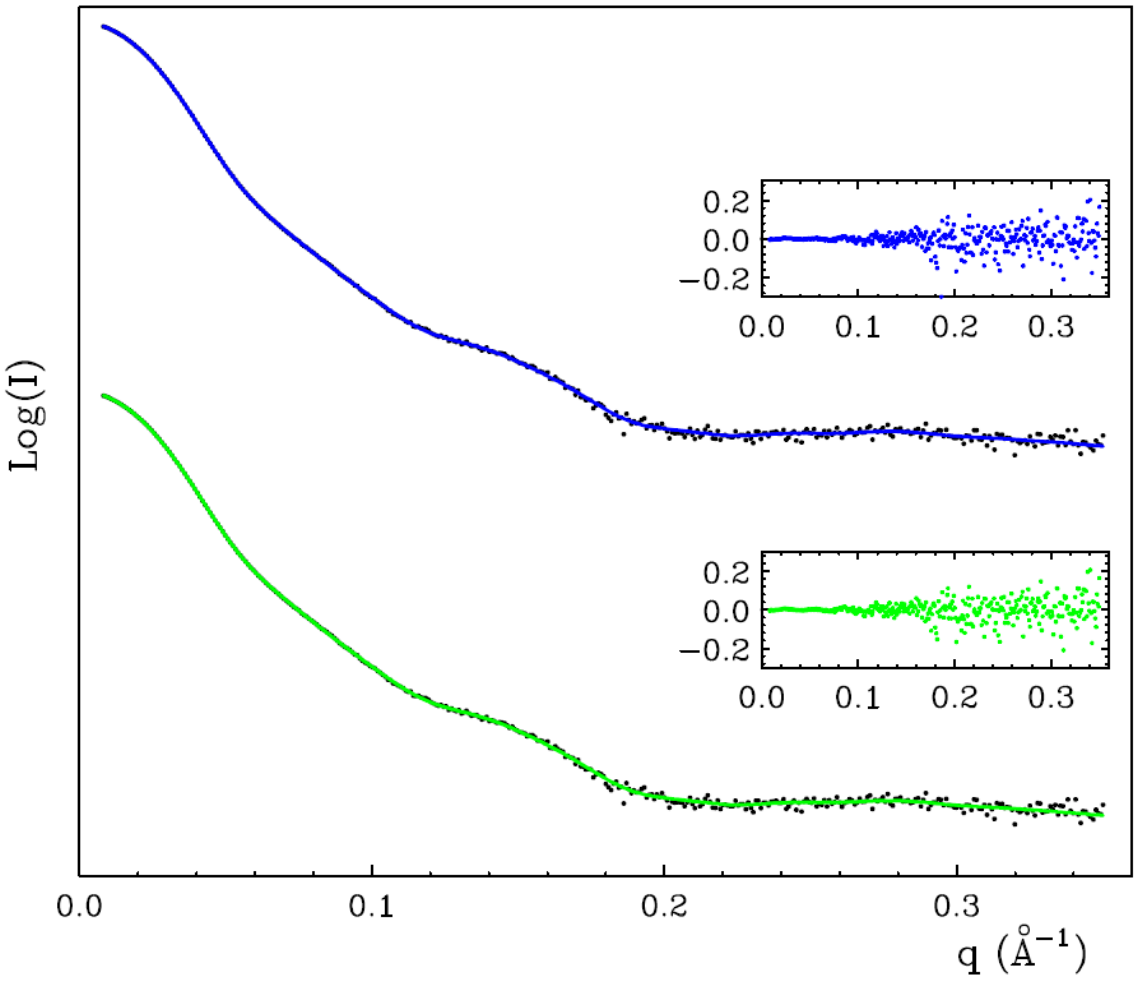

Figure S10

Fit between the experimental data (black dots) and the intensities calculated from the ab-initio model of GAPDH/CP12/PRK complex obtained by DAMMIN (Svergun, 1999) with the default settings (blue line), and with a starting model extracted from rigid-body structures (green line).