

Biophysical Journal, Volume 113

Supplemental Information

**Low-Resolution Structure of Detergent-Solubilized Membrane Proteins
from Small-Angle Scattering Data**

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Supporting Information:

Low Resolution Structure Determination of Detergent Solubilised Membrane Proteins from Small Angle Scattering Data.

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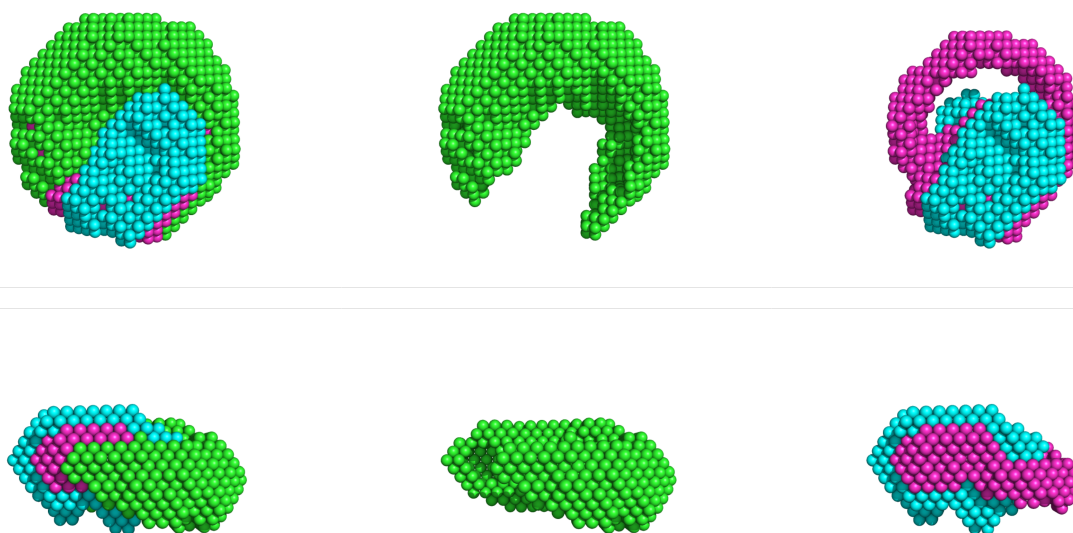


FIG. S1. Ab-initio shape reconstructions of the 270 dDM/AQ0 tetramer using the program MONSA [1], 3 SANS curves as input (0%, 42% and 100% D₂O) and default parameters concerning bead compactness and connectivity, volume fraction and center penalty. Bead colours correspond to: green-protein, cyan - detergent hydrophilic heads and magenta - detergent hydrophobic tails. The volumes of each different phase are provided as input. This is equivalent to providing the detergent aggregation number and head/tail molecular volumes, however the protein volume is an extra parameter that has to be provided to MONSA. The used scattering length densities are the same as those given in Table 1 of the manuscript. Note that due to the similar contrast of detergent heads and protein in all MONSA reconstructions the protein phase beads are positioned erroneously around the detergent tail phase while the detergent head beads form a core close to the centre of the structure. Even considering this core (cyan beads) as the structure representing the protein, we find systematic structural differences ($NSD_{cryst} > 1.0$) comparing to the Aquaporin-0 crystallographic structure. Similar MONSA reconstructions using the two OGD/Fhac experimental SANS curves as input led always to non-physical final shapes for both the protein and the detergent belt.

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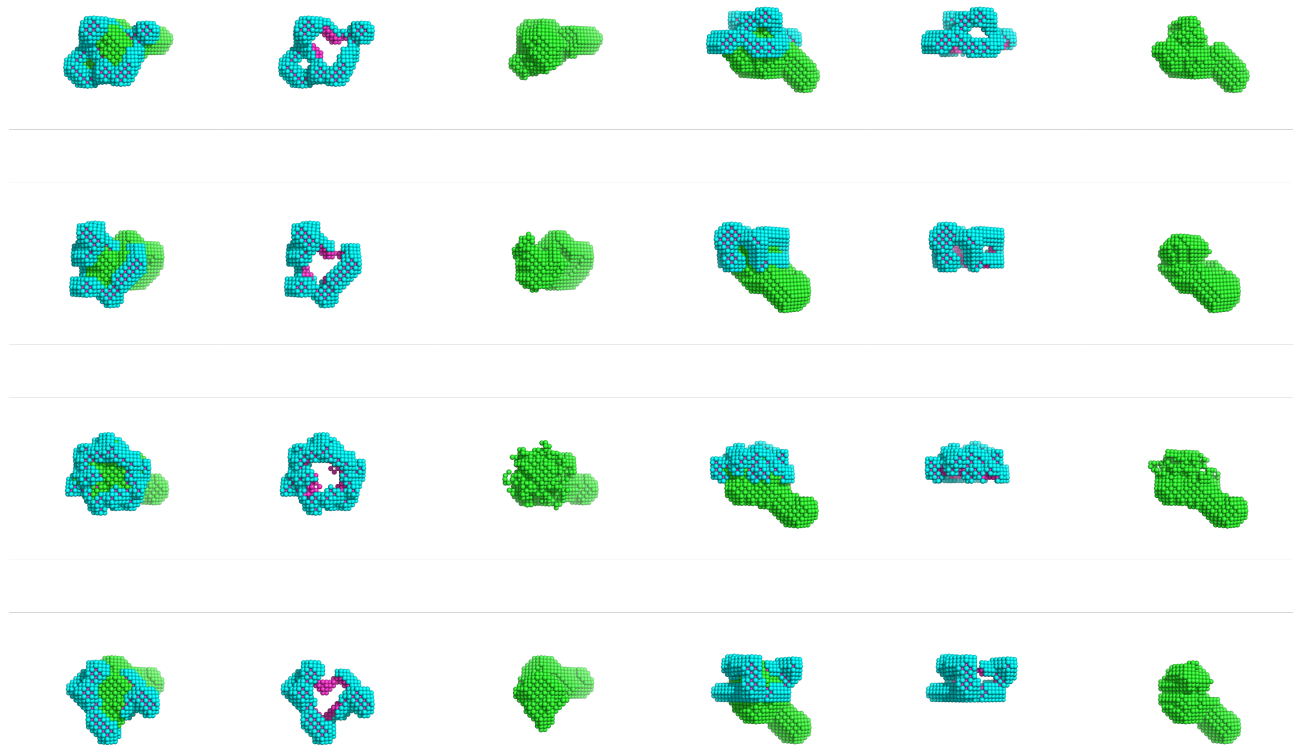


FIG. S2. Results of different ab-initio shape reconstructions of the 140 OG_D/Fhac PDC as the one presented in the manuscript's fig. 4. Each line represents a different ab-initio run. In the first three columns the top view of the different PDC components (entire PDC, detergent belt and protein respectively) are depicted, while in the last three columns the side view. The bead colours correspond to: green - protein, cyan - detergent hydrophilic heads, magenta - detergent hydrophobic tails.

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- [1] Svergun, D. I., 1999. Restoring Low Resolution Structure of Biological Macromolecules from Solution Scattering Using Simulated Annealing. *Biophysical journal* 76:2879–2886.