Congruency between biophysical data from multiple platforms and molecular dynamics simulation of the double super helix model of nascent high-density lipoprotein

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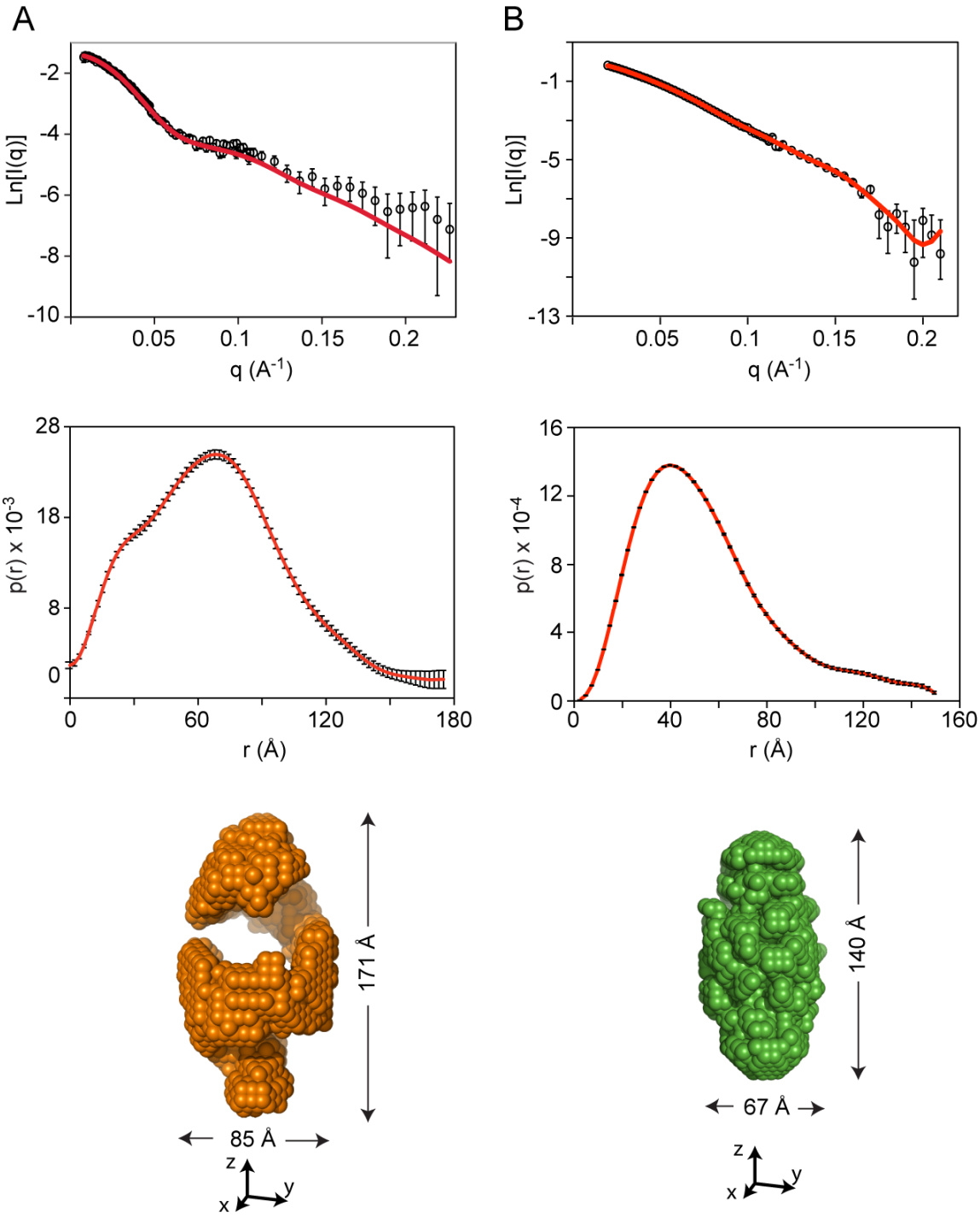
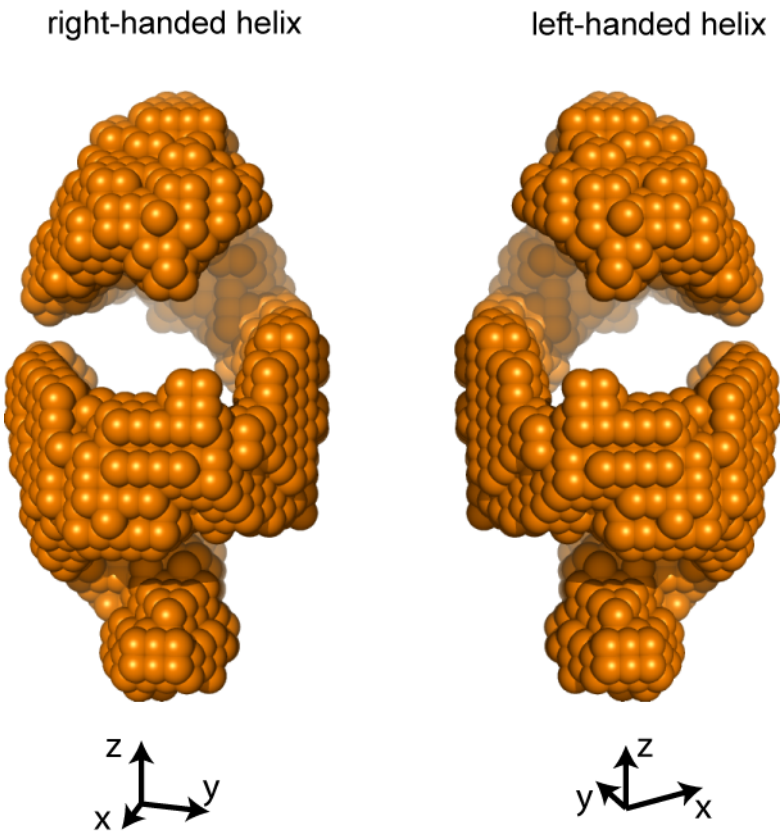
SUPPORTING INFORMATION AVAILABLE

SUPPLEMENTAL FIGURE 1. Small angle neutron scattering intensities and low-resolution structures of nascent rHDL in 12% and 42% D_2O obtained from rHDL analyzed at Münich outstation (FRM-II) of the Jülich Center of Neutron Sciences, Germany. *A*, Top: Small angle neutron scattering intensities of rHDL in 12% D_2O (open circles with error bars), and the calculated scattering intensities from the low-resolution model of apoA1 (red solid line). The calculated curve matches very well the experimental one, which indicates that the 3D arrangement of the scattering centers in the low resolution structure mimics very well the protein conformation; Middle: Distance distribution function, *p(r)*, (red solid line with black error bars) obtained by de-convoluting the scattering intensities. The *p(r)* function is smooth, displays a shoulder around 20 Å, and decays to zero at about 170 Å, which gives the maximum dimension of the protein; Bottom: Low resolution structure of apoA1 in nascent rHDL generated from the *p(r)* function with DANMIN program. The shape is clearly helical and ApoA1 within rHDL is about 170 Å in length and 85 Å in width; *B*, Top: Small angle neutron scattering intensities of nascent rHDL in 42% D_2O (open circles; error bars are not visible) and the calculated scattering intensities from the low-resolution model of the lipid phase in nascent HDL; Middle: Distance distribution function, *p(r)*, (red solid line) obtained by de-convoluting the scattering intensities obtained from HDL samples in 42% D_2O. The *p(r)* function is smooth and decays to zero at about 150 Å, which gives approximately the maximum dimension of the lipid; Bottom: Low resolution structure of the lipid in nascent rHDL. The shape is clearly prolate ellipsoid. The lipid is about 140 Å in length and 67 Å in width.

SUPPLEMENTAL FIGURE 2. Low-resolution structures of nascent rHDL in 12%. **Left:** Right-handed helical conformation of apoA1; **Right:** Left-handed helical conformation of apoA1. The DANMIN program cannot distinguish between mirror images.


A
B
Ln[I(q)]
q (A-1)
p(r) x 10-3
p(r) x 10-4
r (Å)
171 Å
85 Å
140 Å
67 Å
z
y
x


right-handed helix
left-handed helix
z
y
x
z
y
x