

Supporting Information for

## Quaternary structures of GroEL and naïve-Hsp60 chaperones in solution: a combined SAXS-MD study

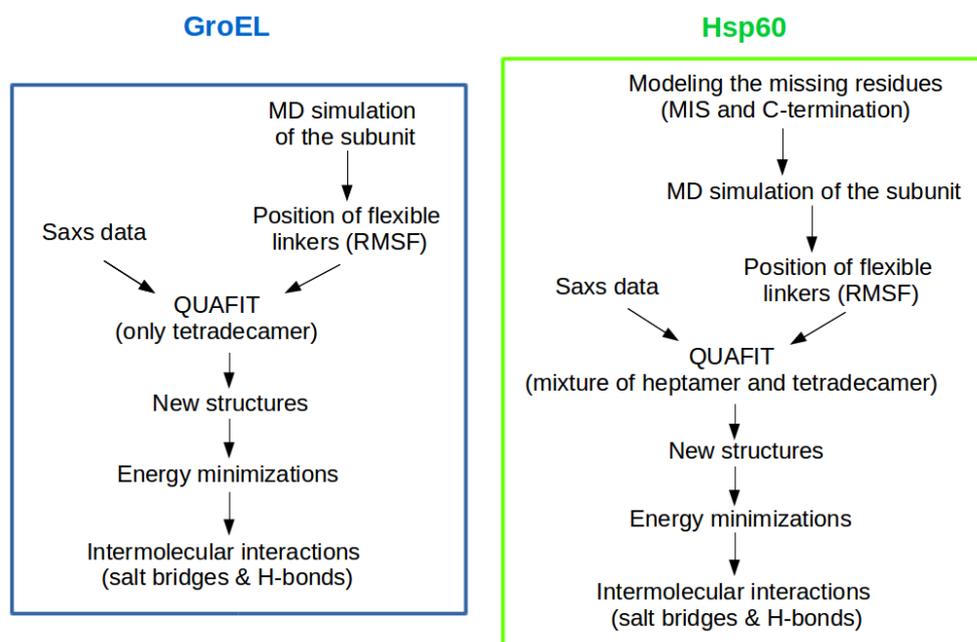
A. Spinello,<sup>a,b</sup> M.G. Ortore,<sup>c\*</sup> F. Spinozzi,<sup>c</sup> C. Ricci,<sup>c</sup> G. Barone,<sup>a,b\*</sup> A. Marino Gammazza,<sup>a,b</sup> and A. Palumbo Piccionello.<sup>a,b\*</sup>

<sup>a</sup> Dipartimento di Scienze e Tecnologie Biologiche, Chimiche e Farmaceutiche-STEBICEF, Viale delle Scienze, Edificio 17, 90128 Palermo, Italy.

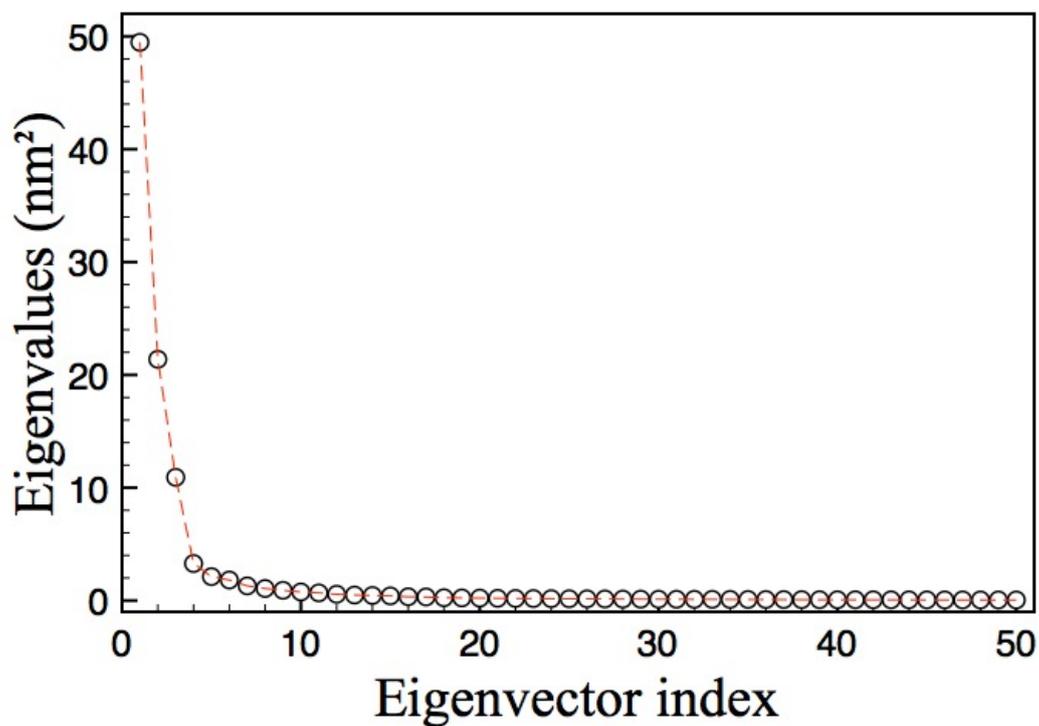
<sup>b</sup> Istituto EuroMediterraneo di Scienza e Tecnologia-IEMEST, Via Emérico Amari 123, 90139 Palermo, Italy.

<sup>c</sup> Dipartimento DiSVA, Università Politecnica delle Marche, via Brecce Bianche, 60131 Ancona, Italy.

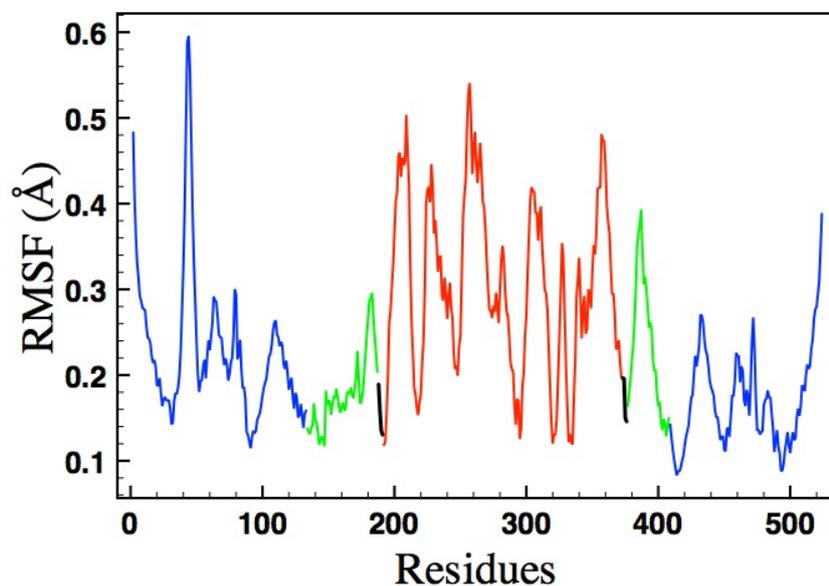
E-mail: [antonio.palumbopiccionello@unipa.it](mailto:antonio.palumbopiccionello@unipa.it), [giampaolo.barone@unipa.it](mailto:giampaolo.barone@unipa.it), [m.g.ortore@univpm.it](mailto:m.g.ortore@univpm.it)



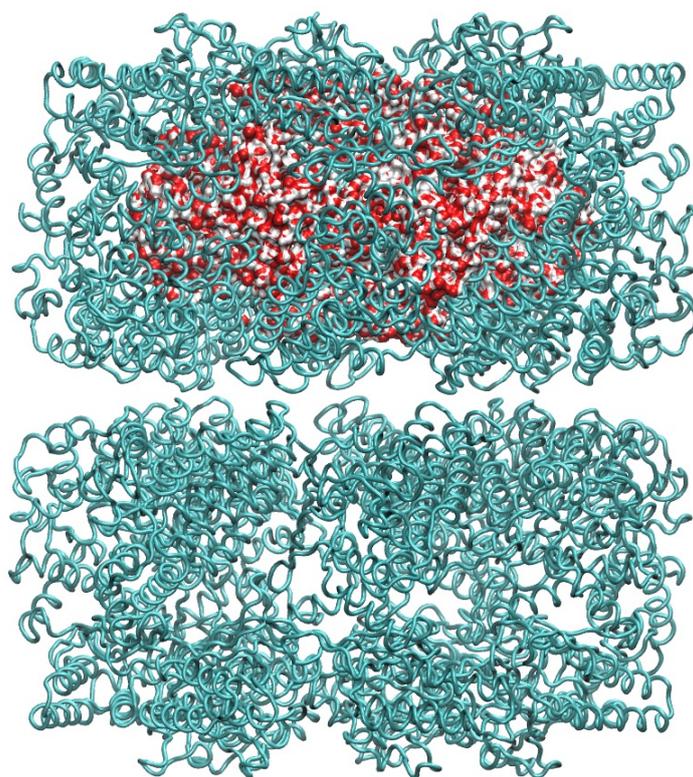
**Figure S1.** Workflow for GroEL (left) and Hsp60 (right)



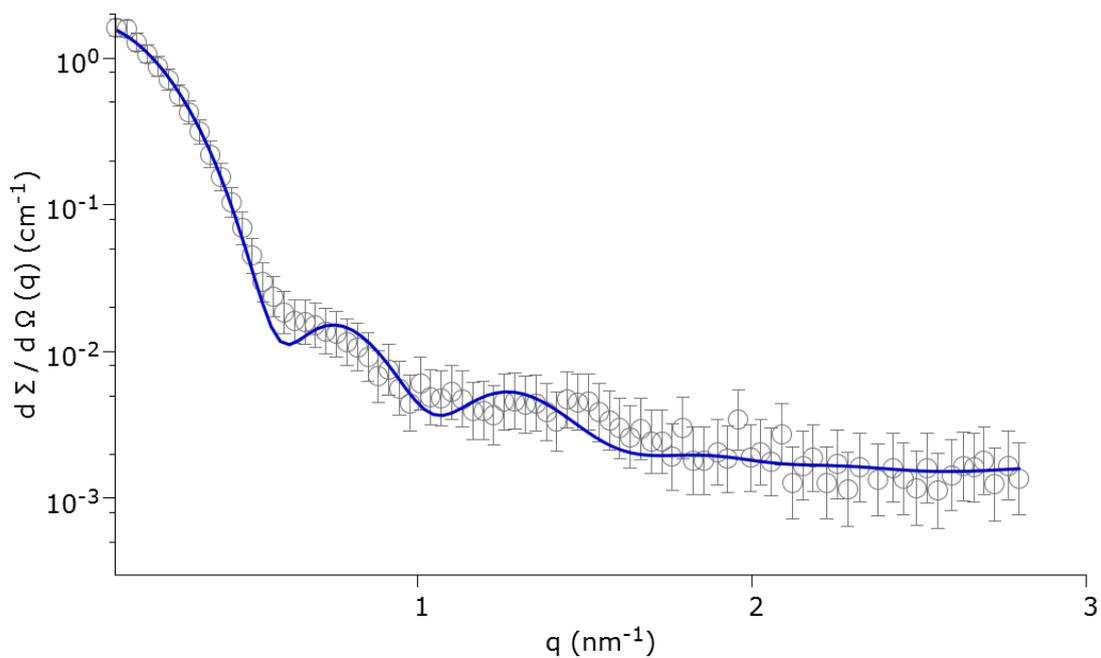
**Figure S2.** Eigenvalues of the first 50 eigenvectors relative to the PCA from 300ns MD of GroEL subunit.



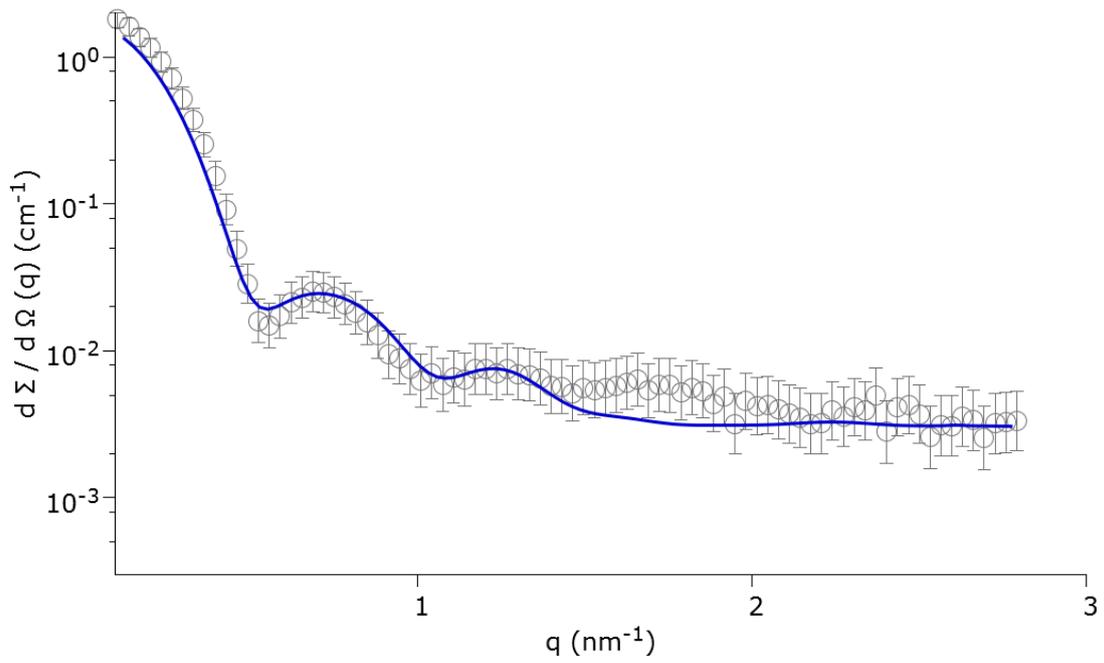
**Figure S3.** Representative residue root mean square fluctuations from 300 ns MD of GroEL. GroEL domains are highlighted by different colors, i.e. equatorial (blue), intermediate (green) and apical (red) domains, respectively. The two flexible linkers are also shown in black.



**Figure S4.** Water molecules inside the single ring (heptamer) cavity of GroEL A structure.



**Figure S5.** SAXS experimental profiles of 3 gL<sup>-1</sup> Hsp60 (open circle), compared with the curves obtained by QUAfit considering only tetradecamers in solution (reduced  $\chi^2=1.81$ ).



**Figure S6.** SAXS experimental profiles of  $3 \text{ gL}^{-1}$  GroEL (open circle), compared with the curves obtained by QUAfit considering the monomer as a single RD (reduced  $\chi^2=2.31$ ).