Supplementary information

Small but large enough: Structural properties of armless mitochondrial tRNAs from the nematode *Romanomermis culicivorax*

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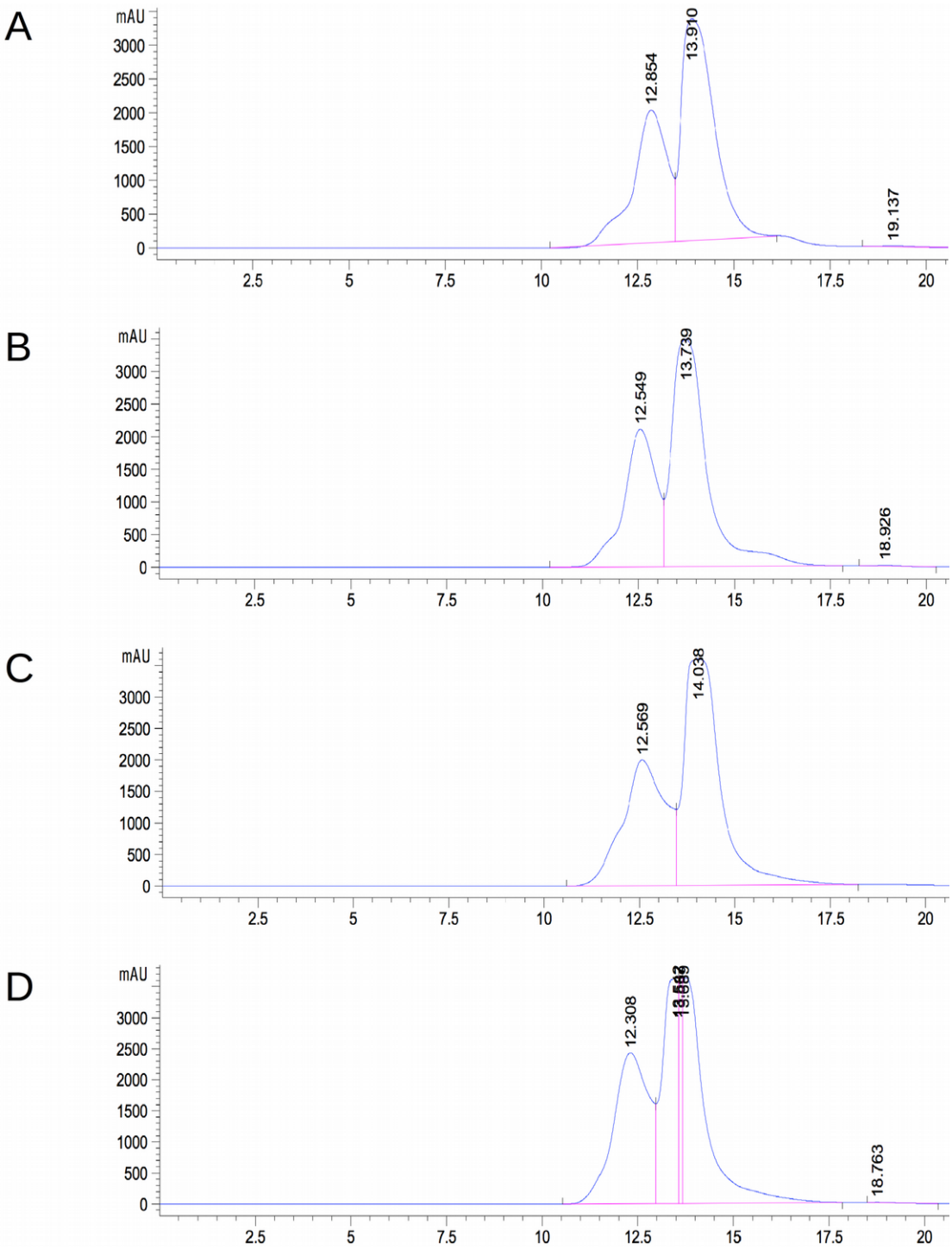

Figure S1. SEC elution of armless tRNAs. Upstream to the SAXS analysis, tRNA samples were eluted on a BIOSEC-3-150 column to separate different populations potentially present in solution. The elution was followed at 280 nm to better distinguish the peaks due to signal saturation at 260 nm. Chromatograms correspond to $tRNA^{Arg}$ in 50 mM HEPES-NaOH pH 7.5, 10 mM MgCl2 (A – low salt) and with 150 KCl (B – high salt), $tRNA^{Ile}$ in 50 mM HEPES-NaOH pH 7.5, 10 mM MgCl2 (C – low salt) and with 150 KCl (D – high salt). In all cases, the major peak corresponding to the monomeric tRNA was preceded by another containing a dimeric form.

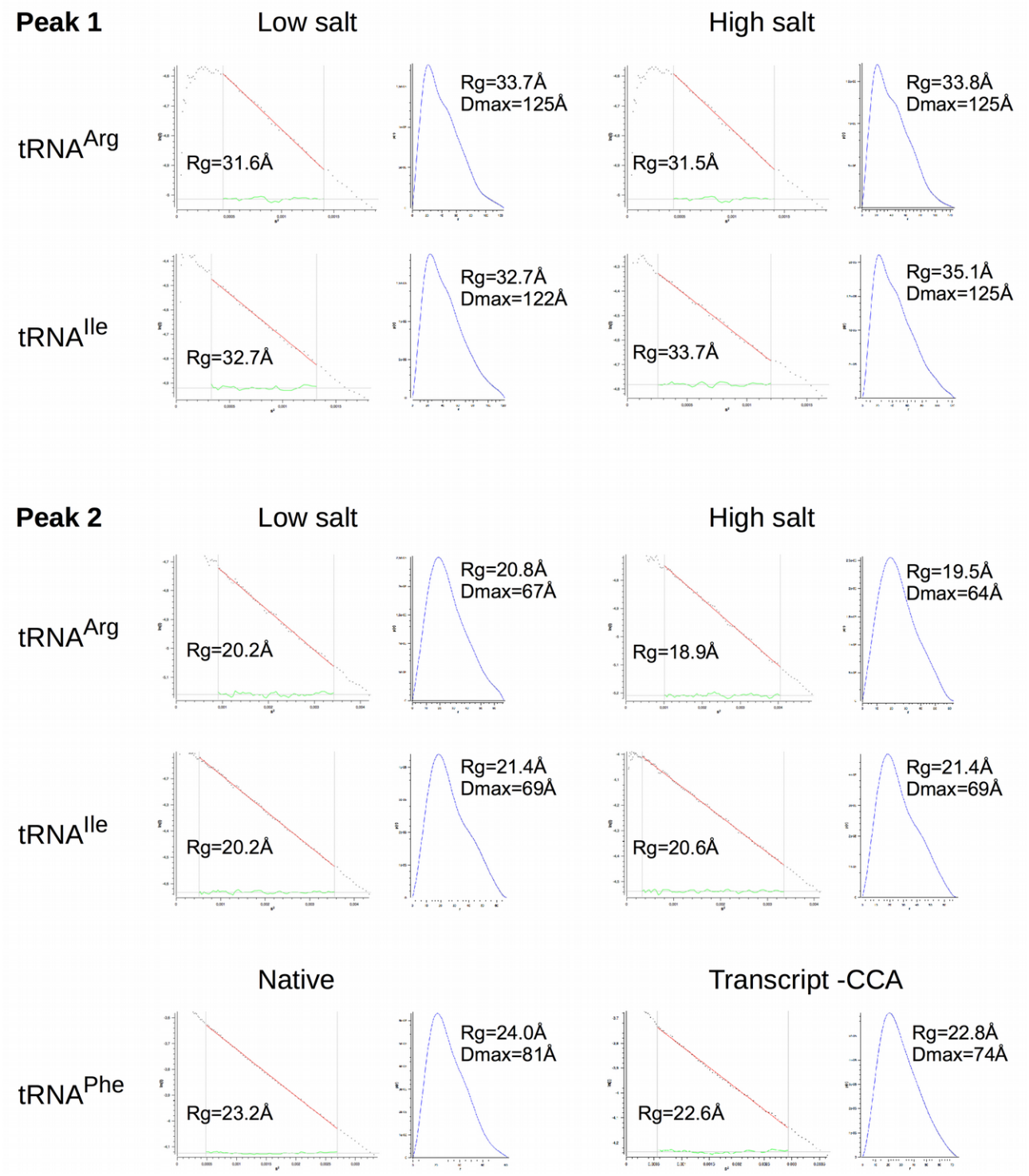

Figure S2. SAXS analysis of armless tRNAs. Guinier plots and p(r) distance distribution functions for each tRNA population isolated by SEC in peaks 1 and 2. The analysis of native yeast $tRNA^{Phe}$ and its transcript deprived of CCA is given for comparison.

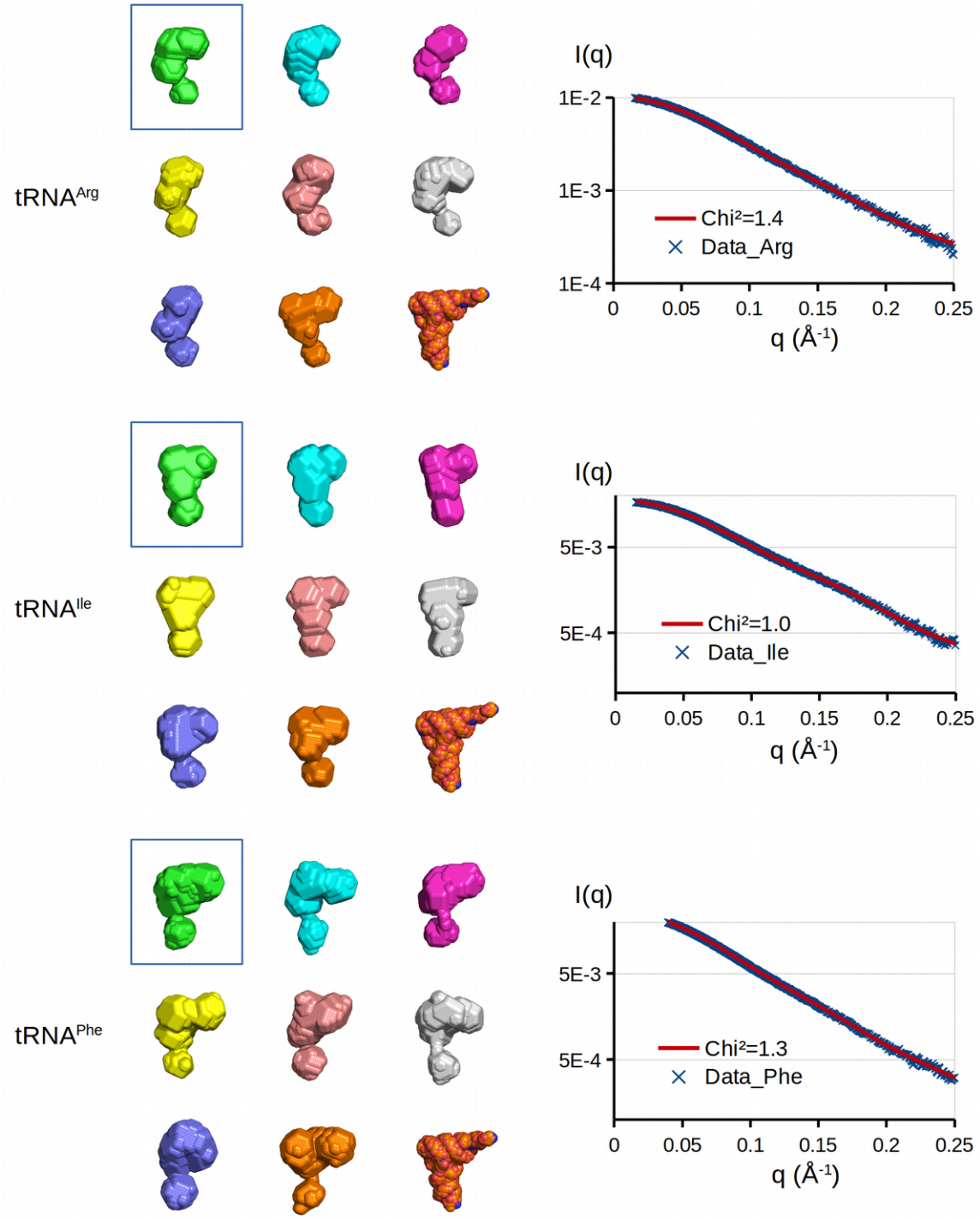

Figure S3. ***Ab initio*** **shape reconstitution of armless tRNAs**. Pseudo-atomic models were derived from SAXS signal with DAMMIF (with q range up to 0.25 $Å^{-1}$) and were superimposed with DAMSUP as described by Franke et al. (2017). Series of representative models are displayed on the left for $tRNA^{Arg}$ (Top), $tRNA^{Ile}$ (Middle) and $tRNA^{Phe}$ (Bottom), together with the crystal structure of the latter (PDBid 1EHZ) for comparison. Central models (i.e. showing the lowest normalized spatial discrepancy) are indicated by a blue box ; corresponding theoretical profile and experimental data are shown on the right in red and blue, respectively, as well as the goodness-of-fit (Chi^2). All models are shown at the same scale.

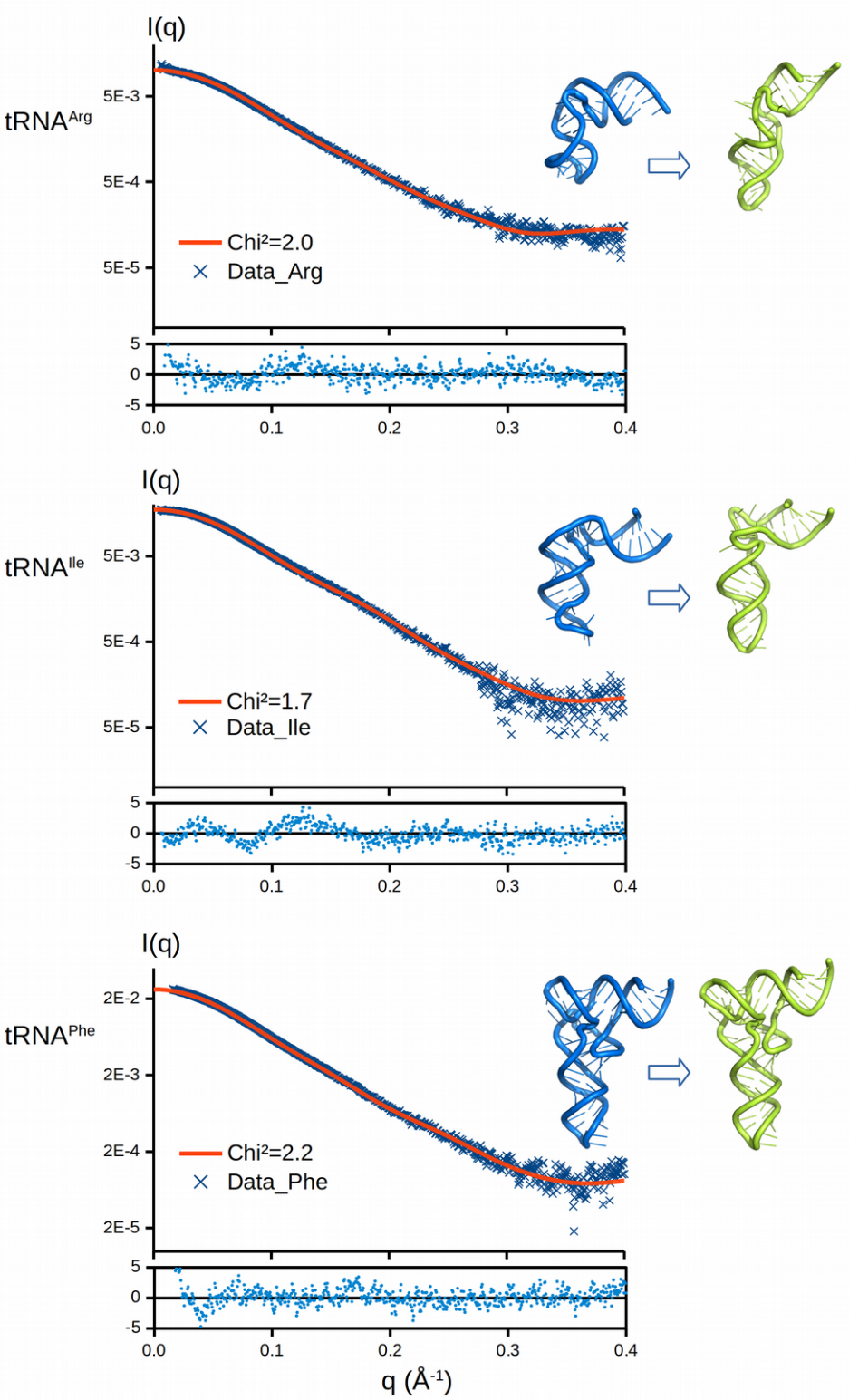

Figure S4. 3D models of armless tRNAs. All-atom models of $tRNA^{Arg}$ and $tRNA^{Ile}$ were built using RNAcomposer (Popenda et al, 2012), whereas the starting model for $tRNA^{Phe}$ was the crystal structure deprived of its CCA tail. The initial models (in blue) were disturbed along their normal modes using ElNemo (Suhre & Sanejouand, 2004) and manually adjusted with SASpy in PyMOL (Panjkovich & Svergun, 2016) to select conformers (in green) that best fitted the SAXS data. Experimental and theoretical profiles, as well as corresponding error-weighted residual difference plot $\Delta/\sigma = [I_{exp}(q) - I_{model}(q)]/\sigma(q)$ and goodness-of-fit (Chi^2), are shown on the left.

References

Franke D, Petoukhov MV, Konarev PV, Panjkovich A, Tuukkanen A, Mertens HDT, Kikhney AG, Hajizadeh NR, Franklin JM, Jeffries CM & Svergun DI (2017), ATSAS 2.8: A comprehensive data analysis suite for small-angle scattering from macromolecular solutions. *J Applied Crystallography* **50:** 1212–1225.

Panjkovich, A. and Svergun, D.I. (2016) SASpy. A PyMOL plugin for manipulation and refinement of hybrid models against small angle X-ray scattering data, *Bioinformatics,* **32,** 2062–2064.

Popenda M, Szachniuk M, Antczak M, Purzycka KJ, Lukasiak P, Bartol N, Blazewicz J, Adamiak RW (2012), Automated 3D structure composition for large RNAs, *Nucleic Acids Res* **40**: e112.

Suhre K & Sanejouand YH (2004), ElNemo: a normal mode web server for protein movement analysis and the generation of templates for molecular replacement. *Nucleic Acids Res* **32**: W610-614.