

**Figure S3. A tetradecamer assembly; Overall architecture, domain organization, and ion-binding.** The SmAP3 14-mer of Fig. S1G is further illustrated in these renditions. As shown in (A), ribbon cartoons that utilize a carefully-chosen color scheme can convey information about both the fold of the SmAP3 monomer, as well as the overall organization of subunits in terms of two SmAP3 heptamers (*apical* and *equatorial*). The two rings – in blue (equatorial) and orange (apical) hues – stack upon one another in a *head–head* manner, but adopt distinct conformations (hence the different hues). Within each ring, an N-terminal domain (NTD) of Sm proteins (orange[api] / blue[equ]) is augmented by C-terminal domains (CTD) that are analogously colored (light orange / light blue). A single subunit of the 14-mer is accentuated in red–yellow, where red corresponds to the NTD<sub>Sm</sub>, and the CTD is yellow. Novel Cd<sup>2+</sup>-binding sites are shown as green spheres, and at successively higher resolution in panels (B) and (C). A rectangular box in (B) indicates the ‘zoomed-in’ region of panel (C). The view in panel (C) is derived from panel (B) by an irregular twist (not a simple rotation), so colors are used to distinguish the two chelating waters (red, violet) and help orient the view. Labels are used to clearly identify relevant molecular entities, such as the amino acid side-chains and water ligands that chelate Cd<sup>2+</sup> in a distorted tetrahedral geometry.

**Figure S4. Volumetric data.** Volumetric quantities, such as electron density or electrostatic potentials, are often the most challenging type of data to illustrate effectively. Chief among the reasons for this is the fact that such data are continuous through 3D space, rather than being discretely ‘chunked’ into atoms, bonds, residues, *etc.*; thus, volumetric data (which generally may be scalar- or vector-valued) are not amenable to representation using the well-established graphical devices of vertices (atoms), lines (bonds), splines (backbone cartoon), triangles (surfaces), and so on. Conventional rendition styles include the isocontour “chicken-wire” meshes that are ubiquitous in crystallography. For instance, an electron density “omit map” at the active site of a *Mycobacterial* dUTPase is shown in (A); note the use of text labels and dashed lines to indicate important structural features of this enzyme. Panels B→E illustrate additional approaches for volumetric data; the utility of each method depends strongly on the specific question addressed by the graphic. For instance, if the aim is to convey information about the electrostatic properties of a molecule, surfaces can be drawn at constant values of the electrostatic potential; these “electrostatic surfaces” are often shown as positive / negative pairs, such as the +3 (blue) and –3 (red)  $k_B T/e$  isocontours shown in (B). However, such images are often quite cluttered, and are therefore of somewhat limited utility. Less ‘busy’ images generally can be attained by mapping the values of the potential onto a surface, such as the solvent-accessible surface or the molecular (Connolly) surface shown in (C). In this example, note the steric *and* electrostatic complementarity between single-stranded poly(A) RNA (sticks) and the surface of the Hfq hexamer. Perhaps the least traditional representation approaches are (i) to directly visualize the field lines corresponding to the gradient of electrostatic potential, as in (D), or (ii) to take a 2D ‘slice’ through 3D volumetric data, as in (E). Volumetric vector fields are often visualized as illuminated streamlines [54]; advanced methods for computation and visualization of such 3D vector fields are beyond the scope of this guide, but recent developments can be found in [55].

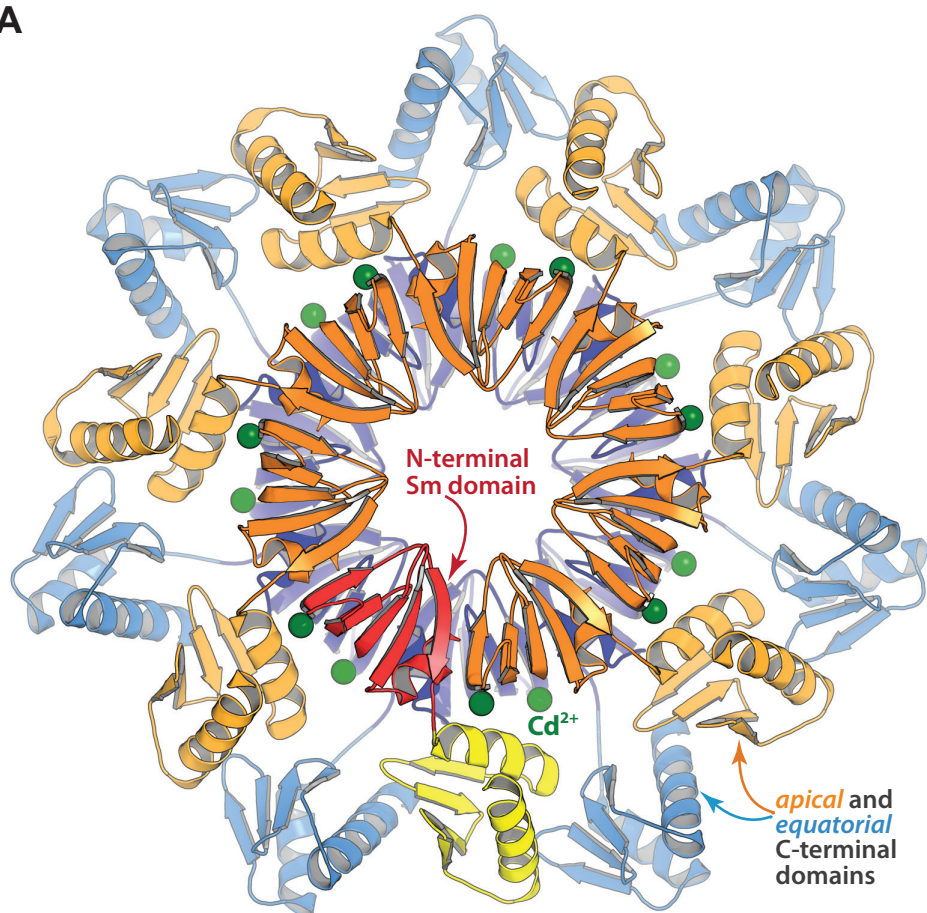
The structure of an *E. coli* Hfq•poly(A) complex was used for the electrostatics calculations illustrated in this figure and in video 2; specific details can be found in the accompanying PyMOL scripts and in the Supplementary Video 2 ‘HowTo’ guide.

**Video S1. DNA helicase.** This animation shows the conformational changes in a helicase as it unwinds double-stranded DNA. The movie is of type  $M_d V_s$  (using the nomenclature of Table 1), and was produced in animated GIF format using PyMOL and the scripts accompanying this primer.

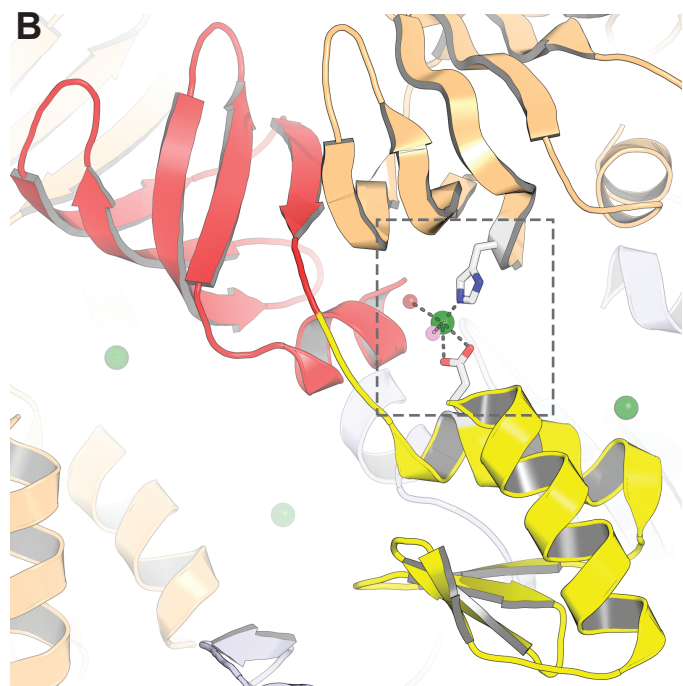
**Video S2. Electrostatics.** This screencast video is a step-by-step demonstration of the usage of PyMOL’s APBS plugin to seamlessly integrate (i) the set-up and execution of a Poisson-Boltzmann electrostatics calculation with (ii) visualization of the resulting grid maps. The steps were performed on a GNU/Linux workstation, using relatively recent releases of the APBS (v1.1) and PyMOL (v1.2) packages.

**Figure S3. A tetradecamer assembly: Overall architecture, bipartite domain organization, and Cd<sup>2+</sup>-binding sites.**

**A**



**B**



**C**

