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Reciprocal space representations of helical objects and their projection images for helices constructed from motifs without spherical symmetry

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Abstract

Formulas for predicting the 3-D reciprocal space cube and 2-D reciprocal space images that are slices of the cube (corresponding to real space images that are projections of the real space cube) are derived for the case when the motif of a helical object is not spherically symmetric. These formulas generalize much-used formulas due to Cochran, Crick, and Vand (*Acta Crystallographica* 5:581–586, 1952) for the case of a spherically-symmetric motif. The new formulas allow control of the spatial resolution of the motif ranging from low-resolution spherically-symmetric motifs as in Cochran, Crick, and Vand through moderate-resolution nonsymmetrical motifs to atomic-resolution nonsymmetrical motifs which can also be treated by the methods of Cochran, Crick, and Vand as a superposition of spherically-symmetric atomic motifs. The ability to control resolution may be useful in reconstruction algorithms analogous to phase extension algorithms in X-ray crystallography.

1 Introduction

Cochran, Crick, and Vand [1] derive formulas for the 3-D reciprocal space cube representation for a helical object which have been extensively used, e.g., [2,3,4], in various tasks, e.g., indexing. These formulas apply in the case when the motif of the helix has spherical symmetry. The purpose of this paper is to generalize these formulas to the case of a motif without spherical symmetry. A key feature of the generalization is that different motifs occur in different orientations, as shown in Fig. 1, which is required if the motif does not have spherical symmetry and has no effect if the motif does have spherical symmetry. The motivation for this generalization is the solution of a statistical 3-D reconstruction problem for helical objects from cryo electron microscope (cryo EM) images analogous to the solution for icosahedrally symmetric objects described in [5,6]. In this approach, a key component is to predict the image that would occur for a particular motif. Roughly analogous to phase extension in X-ray crystallography predictions are initially computed at low resolution but then the resolution is progressively increased. While the formulas of [1] can be used at low resolution, because most

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motifs are roughly spherical at sufficiently low resolution, and can be used at high resolution, because the motif is then a superposition of spherically-symmetric atomic motifs, the new formulas described in this paper are needed at moderate resolutions where the motif is still a smooth density function but no longer has spherical symmetry. While [1] provides formulas for the 3-D reciprocal space cube, additional formulas are provided in this paper for the 2-D reciprocal space image based on the projection-slice theorem. Arbitrary positioning of the helical object in the microscope is allowed. For instance, if the object does not lie flat on the grid of the microscope, then¹ $\beta_L \neq \pi/2$. Similarly, if the object's projection is not aligned with the first component of the real space image coordinate system, then $\gamma_L \neq 0$. Similarly, if the location of the center line of the object's projection is not known, then $x_{L2} \neq 0$. Allowing for $\beta_L \neq \pi/2$, $\gamma_L \neq 0$, and $x_{L2} \neq 0$ makes the resulting formulas complicated. However, if this generality is not needed, then the many trigonometric terms greatly simplify leading to much simpler formulas.

One potential advantage of solving 3-D reconstruction problems in terms of motifs is the ability to include specialized knowledge about the motif, such as symmetry, when such knowledge is available. In this paper that possibility is illustrated by the case of a helical object assembled from bacteriophage P22 polyheads [7] where each polyhead has 6-fold rotational symmetry with a symmetry axis that is radially directed in the helix. A second potential advantage is the ability to use images showing the same motif but in different helical symmetries. Such problems may arise in artificial helical objects, e.g., [8]. We believe that reconstruction algorithms able to solve both of these types of problems can be based on a combination of the models from this paper and the Maximum Likelihood reconstruction tools of [5]. In particular, algorithms of the type described in [5] require the ability to smoothly increase resolution from very low to atomic, as is also common in X-ray crystallography refinement algorithms, and the models of this paper have this characteristic.

The approach of this paper is centered on three coordinate systems. The first coordinate system (so-called motif coordinates) is the system most natural for describing the motif. For instance, in the case where the motif has 6-fold rotational symmetry, a natural coordinate system for a Fourier representation of the motif is one in which the 6-fold axis is the z -axis. The second coordinate system (so-called object coordinates) is a natural system for describing a helical object. In particular, a system where the axis of the helix is the z -axis and a motif is positioned at $(r_H, 0, 0)^T$ in rectangular coordinates, where r_H is the radius of the helix, is used in this paper. The third coordinate system (so-called laboratory coordinates), is the coordinate system such that the projection that creates the image can always be taken to be a z -directed projection. The rotations and translations that connect these coordinate systems will be defined in later sections of the paper. The approach of this paper constructs the helical object in the object coordinate system much as it would be done in a physical system: the motifs are added to the helical object one-by-one with the rotation around the z -axis and the translation along the z -axis relative to the previous motif that is required by the helical symmetry. This contrasts with the approach in [1] in which first a helical wire is defined, then the intersection of the wire with periodically spaced levels is defined, and so forth. Because of the different mechanism of construction, the resulting formulas appear quite different even when the formulas of this paper are specialized to the case of spherically-symmetric motifs. In Section 5 it is demonstrated that the different formulas are, in fact, equivalent when spherically-symmetric motifs are used. In Section 6 a numerical example is presented based on the atomic resolution structure of Tobacco Mosaic Virus (TMV) [9,10,11] which demonstrates the importance of motifs without spherical symmetry for accurate prediction of layer lines.

¹The Euler angles β_L and γ_L and the translation component x_{L2} are defined in the text before Eq. 7.

2 3-D Fourier transform of a helical object

In any of the three reference frames described in the introduction, let $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$ be the unit vectors in the x , y , and z directions of rectangular coordinates for that frame. Let the independent variable in real space be denoted by $\mathbf{x} = (x_1, x_2, x_3)^T \in \mathbf{R}^3$ and the independent variable in 3-D reciprocal space be denoted by $\mathbf{k} = (k_1, k_2, k_3)^T \in \mathbf{R}^3$.

The motif is located at $\mathbf{0}$ in the motif frame and the electron scattering intensity of the motif is denoted by $\rho_M(\mathbf{x})$ and its 3-D Fourier transform, denoted by $P_M(\mathbf{k})$, is defined by $P_M(\mathbf{k}) = \int \rho_M(\mathbf{x}) \exp(-i2\pi\mathbf{k}^T \mathbf{x}) d^3\mathbf{x}$ where superscript T denotes transpose.

In the object frame, the helix has its axis in the $\mathbf{e}_z$ direction and a motif is centered at coordinates $\mathbf{x}_H = r_H \mathbf{e}_x$. Successive motifs are in positions that are shifted by $z_0 \mathbf{e}_z$ and rotated by ϕ_0 . Note that the helix is often described with parameters c , u , and v , where c is the distance along the axial direction per period, u is the number of motifs per period, and v is the number of turns per period. Therefore z_0 and ϕ_0 (for a left-handed helix (Eq. 4)) must satisfy

$$z_0 = \frac{c}{u} \quad (1)$$

$$\phi_0 = \frac{2\pi v}{u} \quad (2)$$

for some $u \in \mathbb{Z}$ and $v \in \mathbb{Z}$ ($\mathbb{Z}$ denotes the integers) where u and v have no common factors [12, Eq. 16]. The helical array of motifs is constructed in two steps. First, a motif is rotated and translated from the motif frame to be centered at position $\mathbf{x}_H$ in the object frame,

$$\rho_{H0}(\mathbf{x}) = \rho_M \left(R_H^{-1} (\mathbf{x} - \mathbf{x}_H) \right), \quad (3)$$

where R_H is the rotation matrix. R_H is described by Euler angles [13, pp. 49–51] denoted by $(\alpha_H, \beta_H, \gamma_H)$. Then the motif is rotated and translated to complete the doubly-infinite helix. In particular, the rotation is in the x - y plane and is described by the rotation matrix S_{ϕ_0} where

$$S_{\phi_0} = \begin{bmatrix} \cos\phi_0 & \sin\phi_0 & 0 \\ -\sin\phi_0 & \cos\phi_0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (4)$$

and the translation is in the z direction and is described by the vector $z_0 \mathbf{e}_z$. Note that $z_0 > 0$ and $\phi_0 > 0$ gives a left-handed helix. The resulting electron scattering intensity of the helical array of motifs in the object frame, denoted by $\rho_H(\mathbf{x})$, is

$$\rho_H(\mathbf{x}) = \sum_{j=-\infty}^{+\infty} \rho_M \left(R_H^{-1} \left[S_{\phi_0}^{-1} (\mathbf{x} - jz_0 \mathbf{e}_z) - \mathbf{x}_H \right] \right). \quad (5)$$

Let $\delta(t)$ be the Dirac delta function. Using the facts that rotation of a real space function implies the same rotation of the corresponding reciprocal space function and that a periodic sequence of delta functions has a Fourier series that is a sum of complex exponentials with equal weights, it can be shown that the 3-D Fourier transform of $\rho_H(\mathbf{x})$, denoted by $P_H(\mathbf{k})$, is²

$$P_H(\mathbf{k}) = \left[\sum_{n=-\infty}^{+\infty} \delta(\mathbf{k}^T u z_0 \mathbf{e}_z - n) \right] \left[\sum_{n'=0}^{u-1} \exp(-i2\pi \mathbf{k}^T [n' z_0 \mathbf{e}_z + S_{n'\phi_0} \mathbf{x}_H]) P_M((S_{n'\phi_0} R_H)^{-1} \mathbf{k}) \right]. \quad (6)$$

Note that Eq. 6 is purely impulsive due to the periodicity of the infinitely long helix.

Transformation from the object frame to the laboratory frame requires both a translation by $\mathbf{x}_L$ and a rotation by R_L which is described in terms of Euler angles denoted by $(\alpha_L, \beta_L, \gamma_L)$. Let the electron scattering intensity of a helical object in the laboratory frame be denoted by $\rho_L(\mathbf{x})$ and its 3-D Fourier transform by $P_L(\mathbf{k})$. Then $P_L(\mathbf{k})$ is

$$\rho_L(\mathbf{x}) = \rho_H(R_L^{-1}(\mathbf{x} - \mathbf{x}_L)) \quad (7)$$

and therefore, by Eq. 3 (Supplement), $P_L(\mathbf{k})$ is

$$P_L(\mathbf{k}) = \exp(-i2\pi \mathbf{k}^T \mathbf{x}_L) P_H(R_L^{-1} \mathbf{k}) \quad (8)$$

$$= \left[\sum_{n=-\infty}^{+\infty} \delta(\mathbf{k}^T u z_0 R_L \mathbf{e}_z - n) \right] \times \left[\sum_{n'=0}^{u-1} \exp(-i2\pi \mathbf{k}^T [\mathbf{x}_L + n' z_0 R_L \mathbf{e}_z + R_L S_{n'\phi_0} \mathbf{x}_H]) P_M((R_L S_{n'\phi_0} R_H)^{-1} \mathbf{k}) \right]. \quad (9)$$

Using the explicit formula for a rotation matrix in terms of Euler angles [13, Eq. 4.43] and $\mathbf{x}_H = (r_H, 0, 0)^T$ gives

$$\begin{aligned} P_L(\mathbf{k}) &= \left[\sum_{n=-\infty}^{+\infty} \delta(k_1 \sin \beta_L \cos \gamma_L - k_2 \sin \beta_L \sin \gamma_L - k_3 \cos \beta_L + \frac{n}{c}) \right] \times \\ &\times \left[\frac{1}{c} \sum_{n'=0}^{u-1} \exp \left(-i2\pi \left[k_1 x_{L1} + k_2 x_{L2} + k_3 x_{L3} + \right. \right. \right. \\ &\quad + n' z_0 (-k_1 \sin \beta_L \cos \gamma_L + k_2 \sin \beta_L \sin \gamma_L + k_3 \cos \beta_L) + \\ &\quad + r_H [k_1 (\cos(\alpha_L + n'\phi_0) \cos \beta_L \cos \gamma_L - \sin(\alpha_L + n'\phi_0) \sin \gamma_L) - \\ &\quad - k_2 (\cos(\alpha_L + n'\phi_0) \cos \beta_L \sin \gamma_L - \sin(\alpha_L + n'\phi_0) \cos \gamma_L) + \\ &\quad \left. \left. + k_3 \cos(\alpha_L + n'\phi_0) \sin \beta_L] \right] \right) P_M((R_L S_{n'\phi_0} R_H)^{-1} \mathbf{k}) \right]. \end{aligned} \quad (10)$$

Note that Eqs. 9 and 10 are purely impulsive for the same reason that Eq. 6 is purely impulsive.

²Please see Supplement Section 1.

3 Image formation model

The image is computed based on the projection-slice theorem in reciprocal space as used in [6, Eq. 1]. Let the independent variable in 2-D real space be denoted by $\chi = (\chi_1, \chi_2)^T \in \mathbb{R}^2$ in rectangular coordinates and the independent variable in 2-D reciprocal space be denoted by $\kappa = (\kappa_1, \kappa_2)^T \in \mathbb{R}^2$ in rectangular coordinates. Let the projection image be denoted by $\sigma(\chi)$ and its Fourier transform by $\Sigma(\kappa)$. The standard first-order thin-sample image formation theory from [14,15] is used. Therefore the image depends only on the projection of the 3-D scattering intensity onto the 2-D plane. Since an arbitrary rotation is included in the transformation from the object frame to the laboratory frame, i.e., Eq. 7, without loss of generality it is assumed that the projection direction is the $\mathbf{e}_z$ direction in the laboratory frame. Combining the first-order thin-sample image formation theory and the projection-slice theorem for projection in the $\mathbf{e}_z$ direction gives

$$\Sigma(\kappa) = G(\kappa) P_L((\kappa^T, 0)^T) \quad (11)$$

where $\kappa = \sqrt{\kappa_1^2 + \kappa_2^2}$ and $G(\kappa)$ is the CTF (Contrast Transfer Function) [16,17].

Combine Eq. 9 or Eq. 10 and Eq. 11 to get

$$\begin{aligned} \Sigma(\kappa) &= G(\kappa) \left[\sum_{n=-\infty}^{+\infty} \delta((\kappa^T, 0) u z_0 R_L \mathbf{e}_z - n) \right] \times \\ &\quad \times \left[\sum_{n'=0}^{u-1} \exp(-i2\pi(\kappa^T, 0) [x_L + n' z_0 R_L \mathbf{e}_z + R_L S_{n' \phi_0} x_H]) \right] \times \\ &\quad \times P_M((R_L S_{n' \phi_0} R_H)^{-1} (\kappa^T, 0)^T) \end{aligned} \quad (12)$$

$$\begin{aligned} &= \left[\sum_{n=-\infty}^{+\infty} \delta\left(\kappa_1 - \kappa_2 \tan \gamma_L + \frac{n}{c \sin \beta_L \cos \gamma_L}\right) \right] \times \\ &\quad \times \frac{G(\kappa) \exp(-i2\pi[\kappa_1 x_{L1} + \kappa_2 x_{L2}])}{c \sin \beta_L \cos \gamma_L} \times \\ &\quad \times \left[\sum_{n'=0}^{u-1} \exp(-i2\pi [n' z_0 (-\kappa_1 \sin \beta_L \cos \gamma_L + \kappa_2 \sin \beta_L \sin \gamma_L) + \right. \\ &\quad \left. + r_H [\kappa_1 (\cos(\alpha_L + n' \phi_0) \cos \beta_L \cos \gamma_L - \sin(\alpha_L + n' \phi_0) \sin \gamma_L) - \right. \\ &\quad \left. - \kappa_2 (\cos(\alpha_L + n' \phi_0) \cos \beta_L \sin \gamma_L + \sin(\alpha_L + n' \phi_0) \cos \gamma_L)] \right] \times \\ &\quad \times P_M((R_L S_{n' \phi_0} R_H)^{-1} (\kappa^T, 0)^T) \end{aligned} \quad (13)$$

Due to the periodicity contained in helical symmetry, Eq. 13 is impulsive, which implies that $\Sigma(\kappa)$ is nonzero only at so-called “layer lines” which occur when κ_1 and κ_2 satisfy $\kappa_1 - \kappa_2 \tan \gamma_L + n/(c \sin \beta_L \cos \gamma_L) = 0$. The in-plane rotation of each layer line is represented by $\tan \gamma_L$ in the reciprocal space image, since γ_L corresponds to rotation around the z axis in the laboratory frame. The spacing between the layer planes in the 3-D cube is the period c but, because of the possibility of out-of-plane tilt, i.e., $\beta_L \neq \pi/2$, the spacing between the layer lines in the 2-D plane is changed to an apparent period $c_a = c \sin \beta_L$.

4 Incorporation of the motif model

The orthonormal expansion model in spherical coordinates described in [5,6] can be used to represent arbitrary electron scattering intensity motifs. The motif, $\rho_M(\mathbf{x})$, is represented as an orthonormal expansion,

$$\rho_M(\mathbf{x}) = \sum_{l=0}^{\infty} \sum_{m=0}^{2l} \sum_{p=1}^{\infty} d_{l,m,p} h_{l,p}(|\mathbf{x}|) \Psi_{l,m}(\theta(\mathbf{x}), \phi(\mathbf{x})), \quad (14)$$

where the unknown weights which determine the 3-D structure of the motif are the $d_{l,m,p}$; the radial basis functions, denoted by $h_{l,p}(\cdot)$ and derived by Sturm-Liouville theory [18, Ch.7], are linear combinations of spherical Bessel functions [19, Eq. 16.9] which satisfy $h_{l,p}(r) = 0$ for $0 \leq r \leq r_1$ and $r_2 \leq r$; and $\Psi_{l,m}(\theta, \phi)$ is a linear combination of spherical harmonics $Y_{l,m}(\theta, \phi)$ [19, Eq. 3.53] chosen so that $\rho_M(\cdot)$ is real for any choice of $d_{l,m,p} \in \mathbb{R}$. The possibility of $r_1 = 0$ is permitted and the possibility of $r_1 = 0$ and $h_{l,p}(0) \neq 0$ for some values of l and p is also permitted. The corresponding 3-D Fourier transform of $\rho_M(\mathbf{x})$, denoted by $P_M(\mathbf{k})$, is

$$P_M(\mathbf{k}) = \sum_{l=0}^{\infty} \sum_{m=0}^{2l} \sum_{p=1}^{\infty} d_{l,m,p} (-i)^l H_{l,p}(|\mathbf{k}|) \Psi_{l,m}(\theta(\mathbf{k}), \phi(\mathbf{k})) \quad (15)$$

where $H_{l,p}(\cdot)$ is the spherical Hankel transform of $h_{l,p}(\cdot)$, which can be computed analytically because of the choice of $h_{l,p}(\cdot)$.

If the motif itself has no particular symmetry, it is sufficient to assume R_H is the identity matrix, denoted by I_3 . By using the orthonormal expansion model for the motif, replacing R_H by I_3 , and using the explicit formula for a rotation matrix in terms of Euler angles, Eq. 10 becomes

$$\begin{aligned} P_L(\mathbf{k}) &= \left[\sum_{n=-\infty}^{+\infty} \delta \left(k_1 \sin \beta_L \cos \gamma_L - k_2 \sin \beta_L \sin \gamma_L - k_3 \cos \beta_L + \frac{n}{c} \right) \right] \times \\ &\times \left[\frac{1}{c} \sum_{l=0}^{\infty} \sum_{m=0}^{2l} \sum_{p=1}^{\infty} d_{l,m,p} (-i)^l H_{l,p}(k') \left[\sum_{n'=0}^{u-1} \exp \left(-i2\pi \left[k_1 x_{L_1} + k_2 x_{L_2} + k_3 x_{L_3} + \right. \right. \right. \right. \\ &\quad \left. \left. \left. + n' z_0 \right) (-k_1 \sin \beta_L \cos \gamma_L + k_2 \sin \beta_L \sin \gamma_L + k_3 \cos \beta_L) + \right. \right. \\ &\quad \left. \left. + r_H \left[k_1 \left(\cos(\alpha_L + n'\phi_0) \cos \beta_L \cos \gamma_L - \sin(\alpha_L + n'\phi_0) \sin \gamma_L \right) - \right. \right. \right. \\ &\quad \left. \left. - k_2 \left(\cos(\alpha_L + n'\phi_0) \cos \beta_L \sin \gamma_L + \sin(\alpha_L + n'\phi_0) \cos \gamma_L \right) + \right. \right. \\ &\quad \left. \left. + k_3 \cos(\alpha_L + n'\phi_0) \sin \beta_L \right] \right) \Psi_{l,m}(\theta', \phi') \right] \end{aligned} \quad (16)$$

where $k' = \sqrt{k_1^2 + k_2^2 + k_3^2}$, $\theta' = \arctan(\sqrt{\mu_1^2 + \mu_2^2}/\mu_3)$, and $\phi' = \arctan(\mu_2/\mu_1)$ and where

$$\begin{aligned} \mu_1(k_1, k_2, k_3) &= k_1 \left[\cos(\alpha_L + n'\phi_0) \cos \beta_L \cos \gamma_L - \sin(\alpha_L + n'\phi_0) \sin \gamma_L \right] \\ &\quad - k_2 \left[\cos(\alpha_L + n'\phi_0) \cos \beta_L \sin \gamma_L - \sin(\alpha_L + n'\phi_0) \cos \gamma_L \right] \\ &\quad + k_3 \cos(\alpha_L + n'\phi_0) \sin \beta_L \end{aligned} \quad (17)$$

$$\begin{aligned}\mu_2(k_1, k_2, k_3) = & k_1 [\sin(\alpha_L + n'\phi_0) \cos \beta_L \cos \gamma_L + \cos(\alpha_L + n'\phi_0) \sin \gamma_L] \\ & + k_2 [-\sin(\alpha_L + n'\phi_0) \cos \beta_L \sin \gamma_L + \cos(\alpha_L + n'\phi_0) \cos \gamma_L] \\ & + k_3 \sin(\alpha_L + n'\phi_0) \sin \beta_L\end{aligned}\quad (18)$$

$$\mu_3(k_1, k_2, k_3) = -k_1 \sin \beta_L \cos \gamma_L + k_2 \sin \beta_L \sin \gamma_L + k_3 \cos \beta_L. \quad (19)$$

Note that $\mu_1^2 + \mu_2^2 = k_1^2 + k_2^2 + k_3^2 - \mu_3^2$.

Similarly, Eq. 13 becomes

$$\begin{aligned}\Sigma(\kappa) = & \left[\sum_{n=-\infty}^{+\infty} \delta \left(\kappa_1 - \kappa_2 \tan \gamma_L + \frac{n}{c \sin \beta_L \cos \gamma_L} \right) \right] \times \\ & \times \frac{G(\kappa) \exp \left(-i2\pi \left[\kappa_1 x_{L1} + \kappa_2 x_{L2} \right] \right)}{c \sin \beta_L \cos \gamma_L} \times \\ & \times \left[\sum_{l=0}^{\infty} \sum_{m=0}^{2l} \sum_{p=0}^{\infty} d_{l,m,p} (-i)^l H_{l,p}(\kappa) \left[\sum_{n'=0}^{u-1} \exp \left(-i2\pi \left[n' z_0 \left(-\kappa_1 \sin \beta_L \cos \gamma_L + \kappa_2 \sin \beta_L \cos \gamma_L \right) \right. \right. \right. \right. \right. \\ & + r_H \left[\kappa_1 \left(\cos(\alpha_L + n'\phi_0) \cos \beta_L \cos \gamma_L - \sin(\alpha_L + n'\phi_0) \sin \gamma_L \right) \right. \\ & \left. \left. - \kappa_2 \left(\cos(\alpha_L + n'\phi_0) \cos \beta_L \sin \gamma_L + \sin(\alpha_L + n'\phi_0) \cos \gamma_L \right) \right] \right] \Psi_{l,m}(\theta, \phi) \right]\end{aligned}\quad (20)$$

where $\kappa = \sqrt{\kappa_1^2 + \kappa_2^2}$, $\theta = \arctan(\sqrt{\tau_1^2 + \tau_2^2}/\tau_3)$, and $\phi = \arctan(\tau_2/\tau_1)$ and where

$$\tau_1(\kappa_1, \kappa_2) = \mu_1(\kappa_1, \kappa_2, 0) \quad (21)$$

$$\tau_2(\kappa_1, \kappa_2) = \mu_2(\kappa_1, \kappa_2, 0) \quad (22)$$

$$\tau_3(\kappa_1, \kappa_2) = \mu_3(\kappa_1, \kappa_2, 0) \quad (23)$$

Note that

$$\tau_1^2 + \tau_2^2 = \kappa_1^2 (\cos^2 \beta_L \cos^2 \gamma_L + \sin^2 \gamma_L) + \kappa_2^2 (\cos^2 \beta_L \sin^2 \gamma_L + \cos^2 \gamma_L) + 2\kappa_1 \kappa_2 \sin^2 \beta_L \cos \gamma_L \sin \gamma_L.$$

If the motif has a known symmetry, then Eq. 14 are overly general and it is likely that a specific orientation of the motif coordinate system will simplify the expression of the symmetric motif. For example, consider the helix assembled from bacteriophage P22 polyheads. Each polyhead has 6-fold rotational symmetry. Such symmetry is most easily expressed if the z axis of the motif coordinate system corresponds to the rotational symmetry axis. In that case, $\Psi_{l,m}(\theta, \phi)$ (Eq. 14) can be written as a linear combination of spherical harmonics $Y_{l,6\eta}(\theta, \phi)$ where $\eta \in \{-L/6, \dots, L/6\}$ (L is the greatest integer less than or equal to l) instead of a linear combination of $Y_{l,s}(\theta, \phi)$ where $s \in \{-l, \dots, l\}$. This implies that the number of basis functions and therefore unknown coefficients is reduced by a factor of 6. However, in the polyhead case,

the rotational symmetry axis is radially directed in the helix, i.e., it lies in the x - y plane ($\beta_H = \pi/2$). Furthermore, if rotation around the rotational symmetry axis is allowed, $\alpha_H \neq 0$. Therefore the motif must be rotated, i.e., $R_H \neq I_3$, but rather

$$R_H = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} \cos \alpha_H & \sin \alpha_H & 0 \\ -\sin \alpha_H & \cos \alpha_H & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (24)$$

$$= \begin{bmatrix} 0 & 0 & -1 \\ -\sin \alpha_H & \cos \alpha_H & 0 \\ \cos \alpha_H & \sin \alpha_H & 0 \end{bmatrix}. \quad (25)$$

This leads to equations analogous to Eqs. 16 and 20, but somewhat more complicated because $R_H \neq I_3$, and therefore not shown.

5 Comparison of the formulas of Cochran, Crick, and Vand [1] with Eq. 6

The formulas of Cochran, Crick, and Vand [1] are based on a spherically-symmetric motif. The methods of [1], if applied to a motif without spherical symmetry, do not yield a helical object because the motif is never rotated, as is shown in Fig. 1. The purpose of this section is to show the equivalence of [1] and a special case of Eq. 6, specifically the case where the motif has spherical symmetry.

The key formula of Cochran, Crick, and Vand, [1, Eqs. (3)–(6)], expressed with delta functions, is

$$F(\mathbf{k}) = \frac{1}{z_0} P_M(|\mathbf{k}|) \sum_{\nu=-\infty}^{+\infty} \sum_{\lambda=-\infty}^{+\infty} \delta(k_z - [\frac{\nu}{z_0} + \frac{\lambda}{P}]) \exp(i\lambda [\Psi - \frac{\pi}{2}]) J_\lambda(2\pi k r_H) \quad (26)$$

where $F(\cdot)$ denotes the 3-D Fourier transform of a left-handed helix in the object frame, $\mathbf{k} = (k, \Psi, k_z)^T$ in cylindrical coordinates, $P_M(\cdot)$ is the 3-D Fourier transform of a spherically-symmetric motif, (so the Fourier transform depends only on the magnitude of the 3-D reciprocal space vector), $P = c/\nu$ which is the pitch of the helix, and $J_\lambda(\cdot)$ is the λ^{th} -order cylindrical Bessel function of the first kind [19, Eq. 3.82]. In Eq. 26, the layer lines are located at those values of k_z such that the argument of the delta function is zero. By substituting $P = c/\nu$ and $z_0 = c/u$,

$$F(\mathbf{k}) = \frac{1}{z_0} P_M(|\mathbf{k}|) \sum_{\nu=-\infty}^{+\infty} \sum_{\lambda=-\infty}^{+\infty} \delta(k_z - \frac{[\nu u + \lambda \nu]}{c}) \exp(i\lambda [\psi - \frac{\pi}{2}]) J_\lambda(2\pi k r_H). \quad (27)$$

In the remainder of this section, the equivalence of Eq. 27, which is essentially from [1], and Eq. 6 is shown for the special case of Eq. 6 where the motif has spherical symmetry. First, as is shown in Supplement Section 2, Eq. 6 is simplified when the motif has spherical symmetry. The result is

$$\begin{aligned}
P_H(\mathbf{k}) &= \frac{1}{c} P_M(|\mathbf{k}|) \sum_{n=-\infty}^{+\infty} \delta\left(k_z - \frac{n}{c}\right) \times \\
&\times \left[\sum_{n'=0}^{u-1} \exp\left(-i2\pi \left[kr_H \cos\left(\frac{2\pi v n'}{u} + \psi\right) + \frac{m n'}{u} \right] \right) \right].
\end{aligned} \tag{28}$$

Second, a major difference between Eqs. 27 and 28 is that Eq. 27 contains a doubly infinite sum (indexed by v, λ) while Eq. 28 has a singly infinite sum and a finite sum (indexed by n, n'). In order to demonstrate the equivalence of Eqs. 27 and 28, it is necessary to change variables of summation in Eq. 27 from v, λ to n, ξ where the relationship between v, λ and n, ξ is shown in Fig. 2. In terms of formulas, it is shown in Supplement Section 3 that there exist integers β and β' such that

$$\sum_{v=-\infty}^{+\infty} \sum_{\lambda=-\infty}^{+\infty} f(v, \lambda) = \sum_{n=-\infty}^{+\infty} \sum_{\xi=-\infty}^{+\infty} f(n\beta' - \xi v, -n\beta + \xi u) \tag{29}$$

for any function $f(\cdot)$ for which the double summation exists. Apply this change of variables to Eq. 27 to get

$$\begin{aligned}
F(\mathbf{k}) &= \frac{1}{z_0} P_M(|\mathbf{k}|) \sum_{n=-\infty}^{+\infty} \sum_{\xi=-\infty}^{+\infty} \delta\left(k_z - \frac{n}{c}\right) \exp\left(i \left[-n\beta + \xi u \right] \left[\Psi - \frac{\pi}{2} \right] \right) J_{-n\beta + \xi u}(2\pi k r_H)
\end{aligned} \tag{30}$$

$$= \frac{1}{z_0} P_M(|\mathbf{k}|) \sum_{n=-\infty}^{+\infty} \delta\left(k_z - \frac{n}{c}\right) \left[\sum_{\xi=-\infty}^{+\infty} \exp\left(i \left[-n\beta + \xi u \right] \left[\Psi - \frac{\pi}{2} \right] \right) J_{-n\beta + \xi u}(2\pi k r_H) \right]. \tag{31}$$

The third step is to use the integral representation of the Bessel function and standard Fourier series results to get³

$$\begin{aligned}
F(\mathbf{k}) &= \frac{1}{c} P_M(|\mathbf{k}|) \sum_{n=-\infty}^{+\infty} \delta\left(k_z - \frac{n}{c}\right) \times \\
&\times \left[\sum_{n'=0}^{u-1} \exp\left(-i2\pi \left[kr_H \cos\left(\frac{2\pi n'}{u} + \Psi\right) - \frac{n\beta n'}{u} \right] \right) \right].
\end{aligned} \tag{32}$$

The remaining difference between Eqs. 28 and 32 is in the summand of the n' summation. The fourth step is to demonstrate that the difference is the order in which the same set of values are enumerated so the sum is the same⁴, i.e.,

³Please see Supplement Section 4.

⁴Please see Supplement Section 5.

$$\begin{aligned}
& \sum_{n'=0}^{u-1} \exp \left(-i2\pi \left[kr_H \cos \left(\frac{2\pi n'}{u} + \Psi \right) + \frac{n\beta n'}{u} \right] \right) \\
&= \sum_{n'=0}^{u-1} \exp \left(-i2\pi \left[kr_H \cos \left(\frac{2\pi n'}{u} + \Psi \right) + \frac{nn'}{u} \right] \right).
\end{aligned} \tag{33}$$

Eq. 33 implies that the results of [1] and the results of this paper when the latter are specialized to the case of spherically-symmetric motifs are identical.

6 Numerical example

In this section a numerical example is presented based on the atomic-resolution structure of Tobacco Mosaic Virus (TMV) [9,10,11].

The spherically-symmetric motif has only $d_{0,0,p}$ nonzero and the values are

$$d_{0,0,p} = \int_0^{r_2} \left[\frac{1}{\sqrt{4\pi}} \int \rho_{\text{TMV}}(\mathbf{x}) d\Omega \right] h_{0,p}(r) r^2 dr \tag{34}$$

where $\rho_{\text{TMV}}(\cdot)$ is the 3-D real space electron scattering intensity of TMV and $\int d\Omega$ means $\int_{\phi=0}^{2\pi} \int_{\theta=0}^{\pi} \sin \theta d\theta d\phi$, i.e., averages over infinitesimally thin spherical shells. The nonsymmetrical motif has all $d_{l,m,p}$ nonzero and the values are

$$d_{l,m,p} = \int_0^{r_2} \left[\int \rho_{\text{TMV}}(\mathbf{x}) \Psi_{l,m}(\theta, \phi) d\Omega \right] h_{l,p}(r) r^2 dr. \tag{35}$$

In both integrals, an impulsive model for the electron scattering intensity of TMV based on atom types (scattering intensities f_j) and locations ($\mathbf{x}_j$) is

$$\rho_{\text{TMV}}(\mathbf{x}) = \sum_{j=1}^J f_j \delta(\mathbf{x} - \mathbf{x}_j) \tag{36}$$

which makes evaluation of the integrals immediate based on exploiting the delta functions. For numerical computation, it is necessary to truncate the l and p sums of Eq. 14, or equivalently Eq. 15. The upper limit is denoted by l_{max} and p_{max} for l and p , respectively. A spherical motif corresponds to $l_{\text{max}} = 0$.

The layer lines for the motif model are computed by Eq. 20 with parameter values listed in Table 1. As described in Table 1, three motif models are considered. The first motif model has spherical symmetry and $p_{\text{max}} = 10$ (spherical symmetry is equivalent to $l_{\text{max}} = 0$), and $d_{0,0,p}$ are computed by Eq. 34. The second and third motif models have no symmetry and $l_{\text{max}} = 6$, $p_{\text{max}} = 10$ and $l_{\text{max}} = 18$, $p_{\text{max}} = 10$, respectively, and $d_{l,m,p}$ are computed by Eq. 35.

The values of $l_{\text{max}} = 18$ and $p_{\text{max}} = 10$ were chosen based on the desire to double the resolution of the model having $l_{\text{max}} = 6$ and $p_{\text{max}} = 10$ and the idea that each $d_{l,m,p}$ makes approximately as much contribution to resolution as one voxel. Therefore, doubling resolution, which requires multiplying the number of voxels by 2^3 , also requires multiplying the number of $d_{l,m,p}$

coefficients, denoted by N_d , by 2^3 . As shown in Table 2, a model with $l_{\max} = 6$, $p_{\max} = 10$ has $N_d = 490$ and a model with $l_{\max} = 18$, $p_{\max} = 10$ has $N_d = 3610$, which is approximately the multiplicative factor desired. In additional calculations (not shown), a model with $l_{\max} = 12$, $p_{\max} = 20$ was considered which has $N_d = 3380$, which is also approximately the multiplicative factor desired. This model had somewhat lower resolution than the $l_{\max} = 18$, $p_{\max} = 10$ model, which we attribute to the highly nonspherical shape of the TMV motif, which leads to more accurate representations when higher l are used.

The layer lines predicted by the three motif models described above are compared with the layer lines predicted by the Protein Data Bank (PDB) atomic-resolution model [9, PDB ID: 2TMV]. The predictions of the atomic-resolution model are computed by applying the formulas of [1] to each spherically-symmetric atom and summing the results. Assume that $\gamma_L = 0$. In particular,

$$\begin{aligned} \Sigma_{\text{atomic}}(\kappa) &= G(\kappa) \exp\left(-i2\pi \left[\kappa_1 x_{L,1} + \kappa_2 x_{L,2} \right]\right) \times \\ &\times \frac{1}{z_0} \sum_{j=1}^J f_j \exp\left(-i2\pi \left[-\kappa_1 \sin \beta_L \right] z_j\right) \times \\ &\times \left[\sum_{\nu=-\infty}^{+\infty} \sum_{\lambda=-\infty}^{+\infty} \delta(-\kappa_1 \sin \beta_L - \left[\frac{\nu}{z_0} + \frac{\lambda}{p} \right]) \exp(i\lambda \left[\Psi' - \phi_j - \frac{\pi}{2} \right]) J_\lambda(2\pi\kappa' r_j) \right] \end{aligned} \quad (37)$$

where the atom locations $\mathbf{x}_j$ (Eq. 36) are in cylindrical coordinates, i.e., (r_j, ϕ_j, z_j) , and

$\kappa' = \sqrt{\kappa_1^2 \cos^2 \beta_L + \kappa_2^2}$, $\Psi' = \tan^{-1}([\sin \alpha_L \cos \beta_L \kappa_1 + \cos \alpha_L \kappa_2] / [\cos \alpha_L \cos \beta_L \kappa_1 - \sin \alpha_L \kappa_2])$, and $\kappa = \sqrt{\kappa_1^2 + \kappa_2^2}$. Fig. 3 shows visualizations of the three motif models and the atomic-resolution PDB model. The spherically-symmetric motif model is shown in the form of electron scattering intensity as a function of radius since the 3-D surface would simply show a sphere.

A variety of methods can be used to specify the resolution of the three motif models. The first method is qualitative comparison of the layer line plots which are shown in Figs. 4 and 5. Note the great qualitative improvement in the similarity of the atomic and the motif layer lines as $l_{\max}$ increases from 0 (spherical model) to 6 (nonspherical model) to 18 (nonspherical model). The same information is shown as diffraction pattern in Fig. 6. Specifically, Fig. 6 shows reciprocal space images (real and imaginary parts) and the magnitude of the reciprocal space images. The reciprocal space images are computed with a sampling interval of $\Delta_s = 0.0017 \text{ \AA}^{-1}$ and the images extend for $\pm 0.2209 \text{ \AA}^{-1}$ (256 pixels) in the direction of the axis of the helix. These parameters control both the number of layer lines that appear in the digital image and the line width of the layer lines. The number of layer lines in the half plane defined by $\kappa_1 \leq 0$ is denoted by $n_{\max}$ and has value $n_{\max} = \lfloor c \times 0.2209 \rfloor + 1 = 16$ although only the first 7 of the layer lines are of sufficient magnitude to be clearly visible in the images, e.g., Fig. 6(l) for the motif without spherical symmetry.

The second method, referred to as the “equal volume” method, compares the number of $d_{l,m,p}$ coefficients in the motif model, i.e., N_d , to the size of the cubic voxels (side dimension of T) required to fill the same volume if the number of voxels is N_d . This implies the formula

$$\frac{4}{3} \pi r_2^3 = T^3 N_d \quad (38)$$

where r_2 is the radius of the sphere in which the motif is nonzero (Eq. 14 and the following description). If T is the sampling interval, then resolution of the motif model is approximately $2T$. These resolution numbers are tabulated in Table 2. In summary, the $l_{\max} = 0, 6, 18$ motif models have resolutions by this measure of 90.34, 24.68, 12.68 Å, respectively.

The third method quantitatively compares the layer lines predicted by each of the three motif models with the layer lines predicted by the atomic-resolution model by a Fourier Ring Correlation (FRC) measure [20]. The definition of FRC is specialized because the layer lines are impulsive. Assume that $\gamma_L = 0$. Write Eq. 20 in the form

$$\sum(\kappa) = \sum_{n=-\infty}^{+\infty} \delta(\kappa_1 + \frac{n}{c \sin \beta_L}) w_n^d(\kappa_2) \quad (39)$$

and similarly for Eq. 37 for the atomic-resolution model but with $w_n^d(\kappa_2)$ replaced by $w_n^a(\kappa_2)$ where “a” stands for “atomic”. The $w_n^d(\kappa_2)$ and $w_n^a(\kappa_2)$ are the weights on the n^{th} layer line. Then define

$$p^{A,B}(\kappa_\alpha, \kappa_\beta) = \sum_n \int_{\kappa_2} w_n^A(\kappa_2) [w_n^B(\kappa_2)]^* d\kappa_2 \quad (40)$$

where $A, B \in \{a, d\}$ and the summation and integration are over the set

$$\left\{ n, \kappa_2 : \kappa_\alpha \leq \sqrt{(n\Delta)^2 + \kappa_2^2} \leq \kappa_\beta \right\} \text{ where } \Delta = 1/c \sin \beta_L \text{ and } \kappa_\alpha \text{ and } \kappa_\beta \text{ are to be specified. Then}$$

$$\text{FRC}(\kappa_\alpha, \kappa_\beta) = \frac{p^{a,d}(\kappa_\alpha, \kappa_\beta)}{\sqrt{p^{a,a}(\kappa_\alpha, \kappa_\beta) p^{d,d}(\kappa_\alpha, \kappa_\beta)}}. \quad (41)$$

The FRC function for the three comparisons of motif models and atomic-resolution model is shown in Fig. 7 where the value of κ_α is $\kappa_\beta - 0.005\text{Å}$ and κ_β ranges from 0.005Å to 0.12Å in steps of size 0.005Å . From these three FRC plots, by using a threshold of 0.5 [21,22], the resolutions of the three models are 59.88Å ($l_{\max} = 0$, spherically-symmetric), 12.82Å ($l_{\max} = 6$, no spherical symmetry), 8.33Å ($l_{\max} = 18$, no spherical symmetry). The improvement in this quantitative measure of resolution matches the qualitative impression from examination of the layer lines shown in Figs. 4 and 5.

7 Conclusion

Formulas for predicting reciprocal space 3-D cubes and 2-D projection images of helical objects constructed from motifs without spherical symmetry were derived. In the case of spherically-symmetric motifs, the formulas reproduce the often-used formulas of Cochran, Crick and Vand [1]. The approach of the paper is to construct a helical object by adding one motif at a time.

In numerical calculation, the infinite sums on the l and p indices in the motif model (Eq. 14) are truncated to $l_{\max}$ and $p_{\max}$, respectively. Different truncations lead to a family of motif

models of varying resolution, including models with spherical symmetry, equivalently, $l_{\max} = 0$.

The motif model is demonstrated with a Tobacco Mosaic Virus (TMV) example. Three motif models, one with spherical symmetry and two without symmetry, are considered. Two quantitative measures of resolution are considered, in addition to the qualitative resolution information provided by plots of the layer lines implied by the motif models. Using Fourier Ring Correlation (FRC) to compare the layer lines implied by the motif models and the layer lines implied by the atomic-resolution model from the PDB indicates that the resolution of the motif models improves from 59.88Å to 12.82Å to 8.33Å as the truncation changes from $l_{\max} = 0, p_{\max} = 10$ to $l_{\max} = 6, p_{\max} = 10$ to $l_{\max} = 18, p_{\max} = 10$. Since only $l_{\max} = 0, p_{\max} = 10$ model has spherical symmetry, this indicates the importance of nonsymmetric motif models, such as described in this paper, if higher resolution is necessary. In addition, the ability to control resolution by altering $l_{\max}$ and $p_{\max}$ is likely important to reconstruction algorithms that describe the helix as an array of motifs and perform refinement as is done in phase extension in X-ray crystallography. Such algorithms might be useful when the motif has a symmetry or when the same motif occurs in objects with different helical symmetries in different images.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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(a) Helical object

(b) The procedure of [1] applied to a motif without spherical symmetry

Figure 1.

A motif without spherical symmetry in an object with helical symmetry (Panel (a)) contrasted with the result of the Cochran, Crick, and Vand [1] procedure (Panel (b)).

Figure 2.
The change in summation variables from v, λ to n, ξ when u is 2 and v is 1. Panel (a): v, λ .
Panel (b): n, ξ .

Figure 3.

Real-space 3-D structure of the motif of TMV. Panel (a): Motif at atomic resolution directly from the PDB coordinates using UCSF Chimera [24]. Panel (b): Spherically-symmetric motif using $l_{\max} = 0, p_{\max} = 10$ which implies 10 $d_{0,0,p}$ coefficients. The motif is shown as a plot of electron scattering intensity versus radius since the 3-D surface is simply a sphere. Panel (c): Motif without symmetry using $l_{\max} = 6, p_{\max} = 10$ which implies 490 $d_{l,m,p}$ coefficients. Panel (d): Motif without symmetry using $l_{\max} = 18, p_{\max} = 10$ which implies 3610 $d_{l,m,p}$ coefficients. The images in both Panels (c) and (d) are from UCSF Chimera [24].

(a) Real part, atomic-resolution model

(b) Real part, spherically-symmetric motif
($l_{\max} = 0, p_{\max} = 10$) (c) Real part, motif without symmetry
($l_{\max} = 6, p_{\max} = 10$)(d) Real part, motif without symmetry
($l_{\max} = 18, p_{\max} = 10$)**Figure 4.**

Real parts of the layer lines of TMV. The layer line number is denoted by n . The value of κ_1 is 0, -0.0145, -0.0290, -0.0435, -0.0580, -0.0725, -0.0870 ($\text{\AA}^{-1}$) corresponding to $n = 0, 1, 2, 3, 4, 5, 6$, respectively. Panel (a): Real part of the layer lines for the atomic-resolution model. Panel (b): Real part of the layer lines for the spherically-symmetric motif using $l_{\max} = 0$, $p_{\max} = 10$ which implies 10 $d_{0,0,p}$ coefficients. Panel (c): Real part of the layer lines for the motif without symmetry using $l_{\max} = 6$, $p_{\max} = 10$ which implies 490 $d_{l,m,p}$ coefficients. Panel (d): Real part of the layer lines for the motif without symmetry using $l_{\max} = 18$, $p_{\max} = 10$ which implies 3610 $d_{l,m,p}$ coefficients.

(a) Imaginary part, atomic-resolution model (b) Imaginary part, spherically-symmetric motif ($l_{\max}=0$, $p_{\max}=10$)

(c) Imaginary part, motif without symmetry ($l_{\max}=6$, $p_{\max}=10$) (d) Imaginary part, motif without symmetry ($l_{\max}=18$, $p_{\max}=10$)

Figure 5.

Imaginary parts of the layer lines of TMV. Panel (a): Imaginary part of the layer lines for the atomic-resolution model. Panel (b): Imaginary part of the layer lines for the spherically-symmetric motif using $l_{\max}=0$, $p_{\max}=10$ which implies 10 $d_{0,0,p}$ coefficients. Panel (c): Imaginary part of the layer lines for the motif without symmetry using $l_{\max}=6$, $p_{\max}=10$ which implies 490 $d_{l,m,p}$ coefficients. Panel (d): Imaginary part of the layer lines for the motif without symmetry using $l_{\max}=18$, $p_{\max}=10$ which implies 3610 $d_{l,m,p}$ coefficients.

Figure 6.

Reciprocal space images for TMV corresponding to the layer lines in Figures 4 and 5. The spherically-symmetric motif has $l_{\max} = 0, p_{\max} = 10$.

Figure 7.

Fourier Ring Correlation (FRC) as a function of κ where FRC is defined in Eq. 41 for three comparisons: Atomic-resolution model versus models with $l_{\max} = 0, p_{\max} = 10$ (10 coefficients), $l_{\max} = 6, p_{\max} = 10$ (490 coefficients), and $l_{\max} = 18, p_{\max} = 10$ (3610 coefficients). The resolution of these three structures are 0.0167, 0.078, and $> 0.12 \text{ \AA}^{-1}$, respectively, or 59.88, 12.82, and $< 8.33 \text{ \AA}$, respectively. The curve for $l_{\max} = 0, p_{\max} = 10$ is truncated at 0. The most negative value is approximately -0.86 near $0.025 \text{ \AA}^{-1}$.

Table 1

Parameter values used in computing the layer lines shown in Figures 4 and 5. The CTF (Contrast Transfer Function) is computed by the formula in [16, 17] where Δf is the deviation from Gaussian focus, C_s is the coefficient of spherical aberration, λ is the electron wavelength, F_{amp} is the fractional amplitude contrast, and B is the decay. Note that negative value of ϕ_0 is used, since TMV is a right-handed helix [9].

	parameter	value		
Rotation (laboratory frame)	α_L	$\pi/6$ (rad)		
	β_L	$\pi/2 - 2\pi/180$ (rad)		
	γ_L	0.0 (rad)		
Translation (laboratory frame)	x_{L1}	0.0 (Å)		
	x_{L2}	0.0 (Å)		
CTF	Δf	1.0×10^4 (Å)		
	C_s	2.0×10^7 (Å)		
	λ	0.0336 (Å)		
	F_{amp}	0.1		
	B	100.0 (Å ²)		
Helical parameters of TMV [9]	c	69.0 (Å)		
	u	49		
	v	3		
	$\phi_0 = -2\pi v/u$	-0.3847 (rad)		
	$z_0 = c/u$	1.4082 (Å)		
	r_H	56.4838 (Å)		
Motif parameters	r_1	0.0 (Å)		
	r_2	60.3670 (Å)		
	l_{max}	0	6	18
	p_{max}	10	10	10

Volume per $d_{l_{m,p}}$ coefficient and motif resolution by equal volume method (Eq. 38) for the motifs with $l_{\max} = 0, 6, 18$ and $p_{\max} = 10$.

Table 2

$l_{\max}$	$p_{\max}$	spherically symmetric	N_d	volume per $d_{l_{m,p}}$ coefficient ($\text{\AA}^3$)	motif resolution by Eq. 38 ($\text{\AA}$)
0	10	Yes	10	$92148.31 = (45.17)^3$	$45.17 \times 2 = 90.34$
6	10	No	490	$1880.58 = (12.34)^3$	$12.34 \times 2 = 24.68$
18	10	No	3610	$255.26 = (6.34)^3$	$6.34 \times 2 = 12.68$