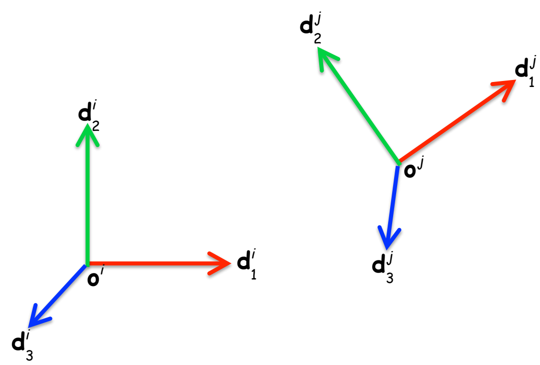
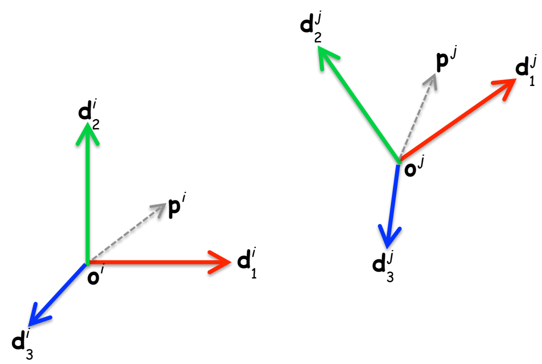
Molecular superposition

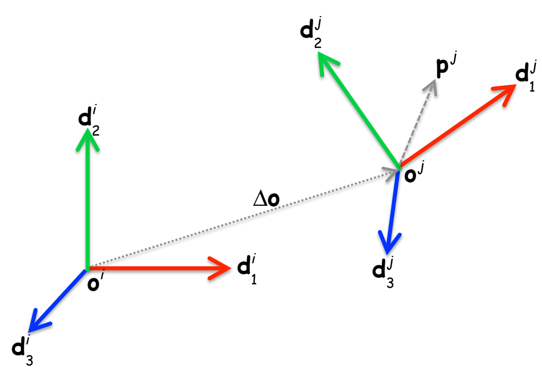
Consider molecular species i and j centered at positions $\mathbf{o}^i$ and $\mathbf{o}^j$ but expressed in different orthogonal reference frames with coordinate axes along unit vectors $\left(\mathbf{d}_1^i, \mathbf{d}_2^i, \mathbf{d}_3^i\right)$ and $\left(\mathbf{d}_1^j, \mathbf{d}_2^j, \mathbf{d}_3^j\right)$.



Comparison of the structures and examination how the position of an arbitrary point $\mathbf{p}^j$ in frame j differs from that of the corresponding atom $\mathbf{p}^i$ in frame i requires a transformation of coordinate frames.

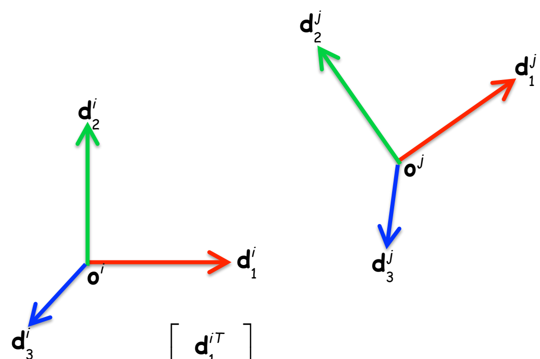


First, the position of the origin $\mathbf{o}^j$ of frame j needs to be expressed in terms of the origin $\mathbf{o}^i$ of frame i, and the coordinates of $\mathbf{p}^j$ in terms of $\mathbf{o}^j$.



Here $\Delta\mathbf{o} = \mathbf{o}^j - \mathbf{o}^i = (x_0, y_0, z_0)$ and $\mathbf{p}^j - \mathbf{o}^j = (x_p, y_p, z_p)$, with the former vector expressed in frame i and the latter in frame j.

The matrix $\mathbf{T}^{ij}$ that effects the coordinate transformation from frame j to frame i can be obtained from the product of a 3×1 pseudovector, or tensor, containing the transposes of the axes of frame i and a 1×3 pseudovector, or tensor, containing the axes of frame j.



$$\mathbf{T}^{ij} = \begin{bmatrix} \mathbf{d}_1^{iT} \\ \mathbf{d}_2^{iT} \\ \mathbf{d}_3^{iT} \end{bmatrix} \begin{bmatrix} \mathbf{d}_1^j & \mathbf{d}_2^j & \mathbf{d}_3^j \end{bmatrix}$$

The $\mathbf{d}_1^i$, $\mathbf{d}_1^i$, $\mathbf{d}_1^i$ are 3×1 column vectors and the $\mathbf{d}_1^j$, $\mathbf{d}_1^j$, $\mathbf{d}_1^j$ are 1×3 row vectors.

The elements of the tensors are unit vectors along the coordinate axes of frames i and j.

$$\mathbf{T}^{ij} = \begin{bmatrix} \mathbf{d}_1^{iT} \\ \mathbf{d}_2^{iT} \\ \mathbf{d}_3^{iT} \end{bmatrix} \begin{bmatrix} \mathbf{d}_1^j & \mathbf{d}_2^j & \mathbf{d}_3^j \end{bmatrix}$$

$$\mathbf{T}^{ij} = \begin{bmatrix} \begin{bmatrix} d_{11}^i & d_{12}^i & d_{13}^i \end{bmatrix} \\ \begin{bmatrix} d_{21}^i & d_{22}^i & d_{23}^i \end{bmatrix} \\ \begin{bmatrix} d_{31}^i & d_{32}^i & d_{33}^i \end{bmatrix} \end{bmatrix} \begin{bmatrix} \begin{bmatrix} d_{11}^j \\ d_{12}^j \\ d_{13}^j \end{bmatrix} & \begin{bmatrix} d_{21}^j \\ d_{22}^j \\ d_{23}^j \end{bmatrix} & \begin{bmatrix} d_{31}^i \\ d_{32}^i \\ d_{33}^i \end{bmatrix} \end{bmatrix}$$

The elements of the resulting 3×3 transformation matrix $\mathbf{T}^{ij}$ are the scalar products of the coordinate axes of frames i and j.

$$\mathbf{T}^{ij} = \begin{bmatrix} \mathbf{d}_1^{iT} \\ \mathbf{d}_2^{iT} \\ \mathbf{d}_3^{iT} \end{bmatrix} \begin{bmatrix} \mathbf{d}_1^{j} & \mathbf{d}_2^{j} & \mathbf{d}_3^{j} \end{bmatrix} = \begin{bmatrix} \sum_{k=i}^{3} d_{1k}^{i} d_{1k}^{j} & \sum_{k=i}^{3} d_{1k}^{i} d_{2k}^{j} & \sum_{k=i}^{3} d_{1k}^{i} d_{3k}^{j} \\ \sum_{k=i}^{3} d_{2k}^{i} d_{1k}^{j} & \sum_{k=i}^{3} d_{2k}^{i} d_{2k}^{j} & \sum_{k=i}^{3} d_{2k}^{i} d_{3k}^{j} \\ \sum_{k=i}^{3} d_{3k}^{i} d_{1k}^{j} & \sum_{k=i}^{3} d_{3k}^{i} d_{2k}^{j} & \sum_{k=i}^{3} d_{3k}^{i} d_{3k}^{j} \end{bmatrix}$$

The elements of the resulting 3×3 transformation matrix $\mathbf{T}^{ij}$ are the scalar products of the coordinate axes of frames i and j.

$$\mathbf{T}^{ij} = \begin{bmatrix} \mathbf{d}_1^{iT} \\ \mathbf{d}_2^{iT} \\ \mathbf{d}_3^{iT} \end{bmatrix} \begin{bmatrix} \mathbf{d}_1^{j} & \mathbf{d}_2^{j} & \mathbf{d}_3^{j} \end{bmatrix} = \begin{bmatrix} \mathbf{d}_1^{i} \cdot \mathbf{d}_1^{j} & \mathbf{d}_1^{i} \cdot \mathbf{d}_2^{j} & \mathbf{d}_1^{i} \cdot \mathbf{d}_3^{j} \\ \mathbf{d}_2^{i} \cdot \mathbf{d}_1^{j} & \mathbf{d}_2^{i} \cdot \mathbf{d}_2^{j} & \mathbf{d}_2^{i} \cdot \mathbf{d}_3^{j} \\ \mathbf{d}_3^{i} \cdot \mathbf{d}_1^{j} & \mathbf{d}_3^{i} \cdot \mathbf{d}_2^{j} & \mathbf{d}_3^{i} \cdot \mathbf{d}_3^{j} \end{bmatrix}$$

Consider the case where the coordinate axes of frame j lie along vectors $\mathbf{d}_1^j = (1,0,0)$, $\mathbf{d}_2^j = (0,1,0)$, and $\mathbf{d}_3^j = (0,0,1)$ and those on frame i lie along $\mathbf{d}_1^i = (d_{11}^i, d_{12}^i, d_{13}^i)$, $\mathbf{d}_2^i = (d_{21}^i, d_{22}^i, d_{23}^i)$, and $\mathbf{d}_3^i = (d_{31}^i, d_{32}^i, d_{33}^i)$.

The matrix $\mathbf{T}^{ij}$ that effects transformation from frame j to frame i is:

$$\mathbf{T}^{ij} = \begin{bmatrix} \mathbf{d}_1^i \cdot \mathbf{d}_1^j & \mathbf{d}_1^i \cdot \mathbf{d}_2^j & \mathbf{d}_1^i \cdot \mathbf{d}_3^j \\ \mathbf{d}_2^i \cdot \mathbf{d}_1^j & \mathbf{d}_2^i \cdot \mathbf{d}_2^j & \mathbf{d}_2^i \cdot \mathbf{d}_3^j \\ \mathbf{d}_3^i \cdot \mathbf{d}_1^j & \mathbf{d}_3^i \cdot \mathbf{d}_2^j & \mathbf{d}_3^i \cdot \mathbf{d}_3^j \end{bmatrix} = \begin{bmatrix} d_{11}^i & d_{21}^i & d_{31}^i \\ d_{12}^i & d_{22}^i & d_{32}^i \\ d_{13}^i & d_{23}^i & d_{33}^i \end{bmatrix}$$

Application of this matrix to the coordinate axes in frame j yields

$$\mathbf{T}^{ij}\mathbf{d}_1^j = \begin{bmatrix} d_{11}^i & d_{21}^i & d_{31}^i \\ d_{12}^i & d_{22}^i & d_{32}^i \\ d_{13}^i & d_{23}^i & d_{33}^i \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} d_{11}^i \\ d_{12}^i \\ d_{13}^i \end{bmatrix}$$

$$\mathbf{T}^{ij}\mathbf{d}_2^j = \begin{bmatrix} d_{11}^i & d_{21}^i & d_{31}^i \\ d_{12}^i & d_{22}^i & d_{32}^i \\ d_{13}^i & d_{23}^i & d_{33}^i \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} d_{21}^i \\ d_{22}^i \\ d_{23}^i \end{bmatrix}$$

$$\mathbf{T}^{ij}\mathbf{d}_3^j = \begin{bmatrix} d_{11}^i & d_{21}^i & d_{31}^i \\ d_{12}^i & d_{22}^i & d_{32}^i \\ d_{13}^i & d_{23}^i & d_{33}^i \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} d_{31}^i \\ d_{32}^i \\ d_{33}^i \end{bmatrix}$$

In other words, the coordinate axes of frame j coincide with those of frame i.

Similarly consider the case where the coordinate axes of frame i lie along vectors $\mathbf{d}^i_1=\left(1,0,0\right)$, $\mathbf{d}^i_2=\left(0,1,0\right)$, and $\mathbf{d}^i_3=\left(0,0,1\right)$ and those on frame j lie along $\mathbf{d}^j_1=\left(d^j_{11},d^j_{12},d^j_{13}\right)$, $\mathbf{d}^j_2=\left(d^j_{21},d^j_{22},d^j_{23}\right)$, and $\mathbf{d}^j_3=\left(d^j_{31},d^j_{32},d^j_{33}\right)$.

$$\mathbf{T}^{ji}=\mathbf{T}^{ij^T}=\begin{bmatrix}\mathbf{d}^i_1\cdot\mathbf{d}^j_1 & \mathbf{d}^i_2\cdot\mathbf{d}^j_1 & \mathbf{d}^i_3\cdot\mathbf{d}^j_2\\ \mathbf{d}^i_1\cdot\mathbf{d}^j_2 & \mathbf{d}^i_2\cdot\mathbf{d}^j_2 & \mathbf{d}^i_3\cdot\mathbf{d}^j_2\\ \mathbf{d}^i_1\cdot\mathbf{d}^j_3 & \mathbf{d}^i_2\cdot\mathbf{d}^j_3 & \mathbf{d}^i_3\cdot\mathbf{d}^j_3\end{bmatrix}=\begin{bmatrix}d^j_{11} & d^j_{21} & d^j_{31}\\ d^j_{12} & d^j_{22} & d^j_{32}\\ d^j_{13} & d^j_{23} & d^j_{33}\end{bmatrix}$$

The matrix $\mathbf{T}^{ji}$ that effects the coordinate transformation from frame i to j is the transpose of the matrix $\mathbf{T}^{ij}$ that effects the coordinate transformation from frame j to i.

Application of the transposed matrix to the coordinate axes in frame i yields

$$\mathbf{T}^{ji}\mathbf{d}^i_1=\begin{bmatrix}d^j_{11} & d^j_{21} & d^j_{31}\\ d^j_{12} & d^j_{22} & d^j_{32}\\ d^j_{13} & d^j_{23} & d^j_{33}\end{bmatrix}\begin{bmatrix}1\\0\\0\end{bmatrix}=\begin{bmatrix}d^j_{11}\\ d^j_{12}\\ d^j_{13}\end{bmatrix}$$

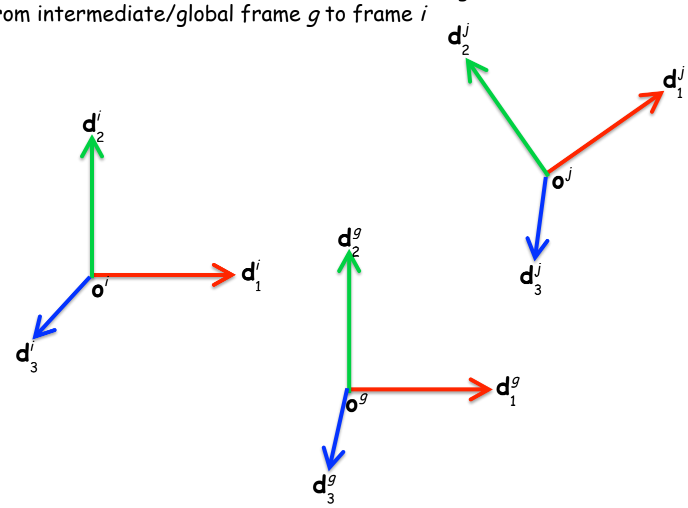
$$\mathbf{T}^{ji}\mathbf{d}^i_2=\begin{bmatrix}d^j_{11} & d^j_{21} & d^j_{31}\\ d^j_{12} & d^j_{22} & d^j_{32}\\ d^j_{13} & d^j_{23} & d^j_{33}\end{bmatrix}\begin{bmatrix}0\\1\\0\end{bmatrix}=\begin{bmatrix}d^j_{21}\\ d^j_{22}\\ d^j_{23}\end{bmatrix}$$

$$\mathbf{T}^{ji}\mathbf{d}^i_3=\begin{bmatrix}d^j_{11} & d^j_{21} & d^j_{31}\\ d^j_{12} & d^j_{22} & d^j_{32}\\ d^j_{13} & d^j_{23} & d^j_{33}\end{bmatrix}\begin{bmatrix}0\\0\\1\end{bmatrix}=\begin{bmatrix}d^j_{31}\\ d^j_{32}\\ d^j_{33}\end{bmatrix}$$

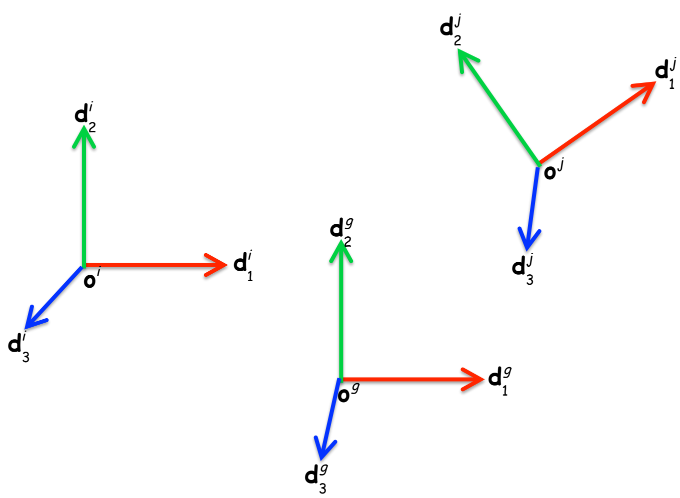
Now the coordinate axes of frame i coincide with those of frame j.

The transformation from frame j to frame i can be thought of as a two-step transformation

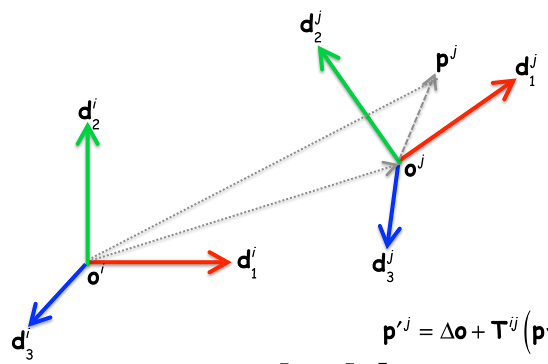
(1) from frame j to an intermediate/global frame g with unit vectors (1,0,0), (0,1,0), and (0,0,1) along the coordinate axes
(2) from intermediate/global frame g to frame i



Alternatively, frame j and frame i can be separately transformed to the common global frame.



The coordinates of position $\mathbf{p}^j$ in frame i is a sum of two vectors: the vector $\Delta\mathbf{o}=(\mathbf{o}^j - \mathbf{o}^i)$ joining the origins $\mathbf{o}^i$ and $\mathbf{o}^j$ and the transformed vector $\mathbf{T}^{ij}(\mathbf{p}^j - \mathbf{o}^j)$ connecting $\mathbf{o}^j$ to $\mathbf{p}^j$.



$$\mathbf{p}'^j = \Delta\mathbf{o} + \mathbf{T}^{ij}\left(\mathbf{p}^j - \mathbf{o}^j\right)$$

$$= \begin{bmatrix} x_0 \\ y_0 \\ z_0 \end{bmatrix} + \begin{bmatrix} \mathbf{d}_1^i\cdot\mathbf{d}_1^j & \mathbf{d}_1^i\cdot\mathbf{d}_2^j & \mathbf{d}_1^i\cdot\mathbf{d}_3^j \\ \mathbf{d}_2^i\cdot\mathbf{d}_1^j & \mathbf{d}_2^i\cdot\mathbf{d}_2^j & \mathbf{d}_2^i\cdot\mathbf{d}_3^j \\ \mathbf{d}_3^i\cdot\mathbf{d}_1^j & \mathbf{d}_3^i\cdot\mathbf{d}_2^j & \mathbf{d}_3^i\cdot\mathbf{d}_3^j \end{bmatrix} \begin{bmatrix} x_p \\ y_p \\ z_p \end{bmatrix}$$

The 3D coordinate transformation can be written in terms of a 2×2 generator matrix and 2×1 vector, both tensors, with matrix/vector elements

$$\begin{bmatrix} \mathbf{p}'^j \\ 1 \end{bmatrix} = \begin{bmatrix} \mathbf{T}^{ij} & \Delta\mathbf{o} \\ \mathbf{0} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{p}^j - \mathbf{o}^j \\ 1 \end{bmatrix}$$

or in terms of a 4×4 generator matrix and 4×1 vector with scalar elements

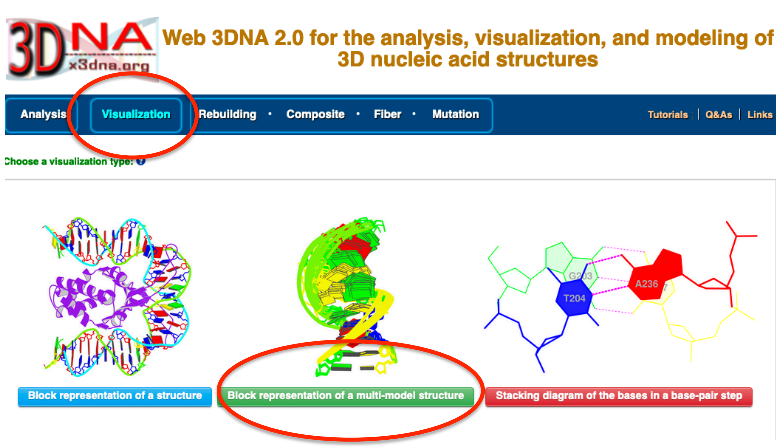
$$\begin{bmatrix} x'_p \\ y'_p \\ z'_p \\ 1 \end{bmatrix} = \begin{bmatrix} \mathbf{d}_1^i\cdot\mathbf{d}_1^j & \mathbf{d}_1^i\cdot\mathbf{d}_2^j & \mathbf{d}_1^i\cdot\mathbf{d}_3^j & x_0 \\ \mathbf{d}_2^i\cdot\mathbf{d}_1^j & \mathbf{d}_2^i\cdot\mathbf{d}_2^j & \mathbf{d}_2^i\cdot\mathbf{d}_3^j & y_0 \\ \mathbf{d}_3^i\cdot\mathbf{d}_1^j & \mathbf{d}_3^i\cdot\mathbf{d}_2^j & \mathbf{d}_3^i\cdot\mathbf{d}_3^j & z_0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_p \\ y_p \\ z_p \\ 1 \end{bmatrix}$$

Here $\Delta\mathbf{o} = \mathbf{o}^j - \mathbf{o}^i = (x_0, y_0, z_0)$ and $\mathbf{p}^j - \mathbf{o}^j = (x_p, y_p, z_p)$, with the former vector expressed in frame i and the latter in frame j. The boldface $\mathbf{0}$ in the top expression is a row vector of order 1×3 with null elements.

w3DNA application

Visualization: block representation of an ensemble of structures

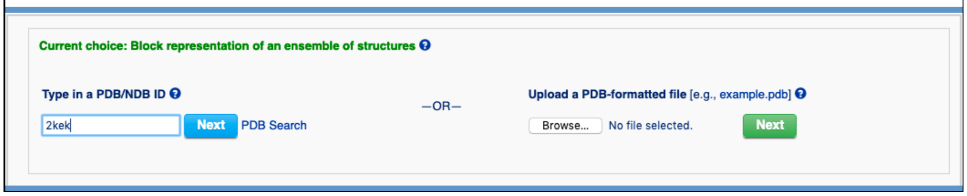
http://web.x3dna.org/



A base-pair superposition option can be reached by first choosing **Visualization** at the main page site and then **Block representation •••** at the Visualization page.

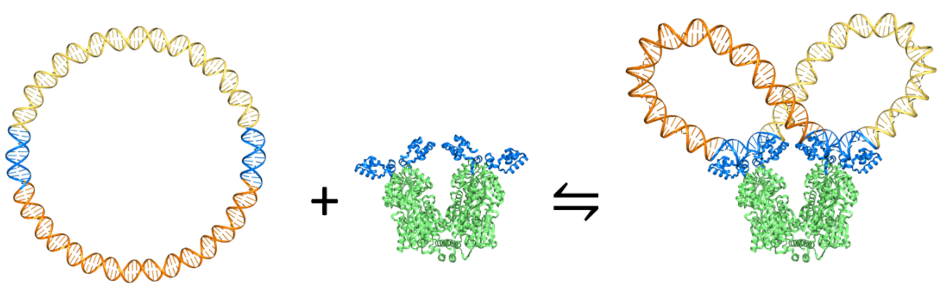
Protein Data Bank file 2kek contains the coordinates of 10 nmr models of the complex of the Lac repressor protein headpiece and the *O*3 DNA operator.

Romanuka, J., Folkers, G.E., Biris, N., Tishchenko, E., Wienk, H., Bonvin, A.M.J.J., Kaptein, R., & Boelens, R. Specificity and affinity of Lac repressor for the auxiliary operators *O2* and *O3* are explained by the structures of their protein-DNA complexes. *J. Mol. Biol.* **390**, 478-489 (2009)



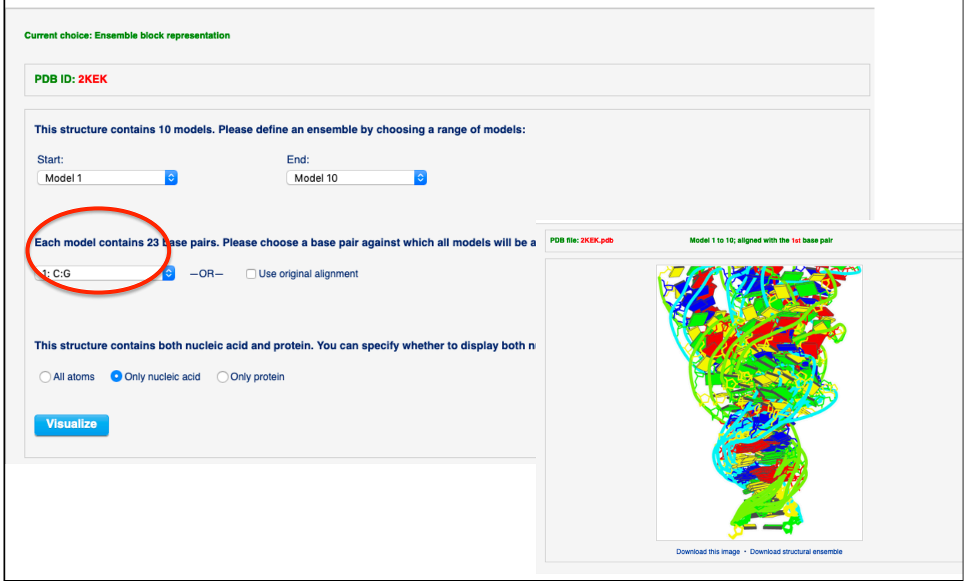
The Lac repressor is the classic textbook example of a protein that attaches to widely spaced sites along DNA and forces the intervening residues into a loop.

The loops induced by the binding of the repressor to operator sites on the *Escherichia coli* genome are thought to impede the synthesis of gene products. Here we illustrate Lac-repressor-mediated loops formed on a small DNA minicircle.

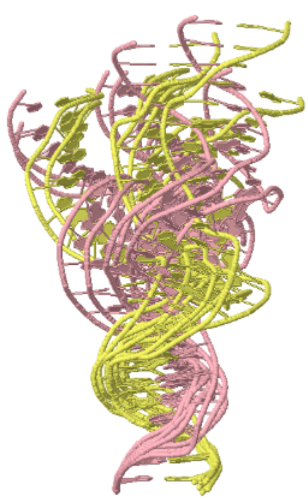


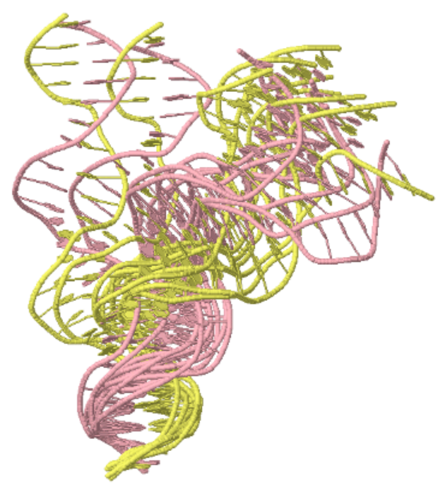
Perez & Olson (2016) Biophys Revs

The differences among the models are striking when the DNA chains are superimposed on the terminal base pairs, here the first base pair.



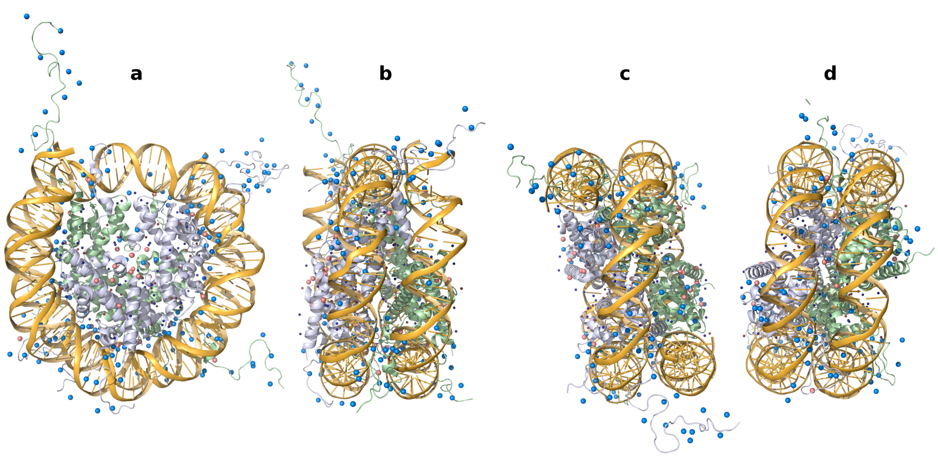
The JSmol option allows the user to select specific structural models and molecular species (here all 10 models of DNA only) and to see spinning images.





Nucleosome superposition

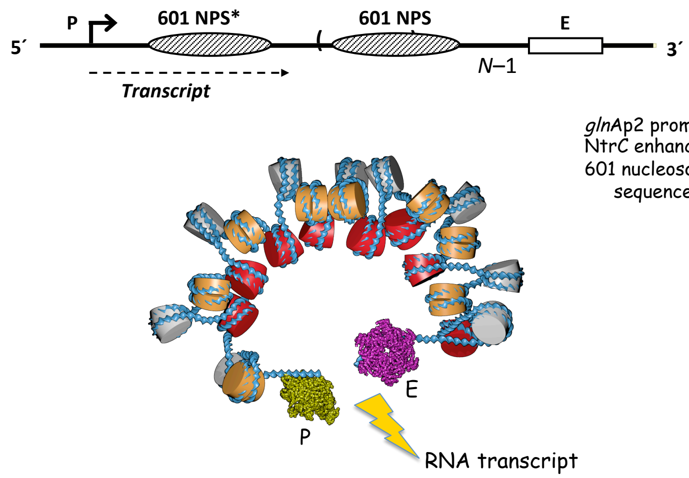
The nucleosome is the fundamental packaging unit of DNA in chromatin.



Orthogonal views of the 1.9-Å core-particle structure (pdb id 1kx5) bearing human α-satellite DNA.

Davey et al. (2002) Solvent mediated interactions in the structure of the nucleosome core particle at 1.9 Å resolution, J Mol Biol 319, 1097-1111.

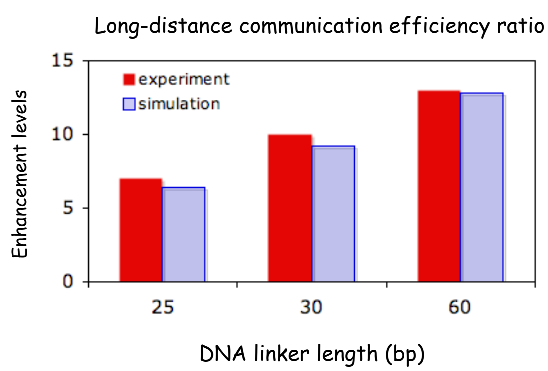
The level of gene products formed upon the association of transcriptional proteins, bound at the ends of a saturated, nucleosome-decorated DNA array, provides a novel measure of the looping propensities of chromatin.



*gln*Ap2 promoter – P
NtrC enhancer - E
601 nucleosome-positioning sequence - NPS

Vasily Studitsky lab

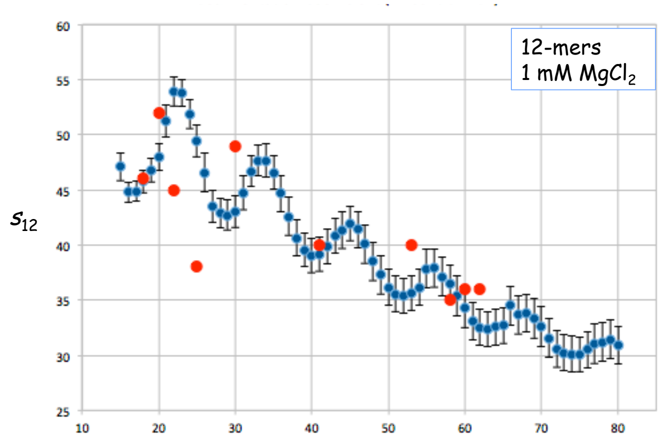
Simulations of nucleosome-decorated DNA arrays account for effects of DNA linker length on long-distance communication efficiency.



Observed and simulated values of enhancer-promoter communication along constructs with 13 intervening nucleosomes and internucleosomal dyad spacing of 172, 177, and 207 bp.

Nizovtseva et al (2017) Nucleosome-free DNA regions differentially affect distant communication in chromatin. Nucleic Acids Res 45(6):3059-3067 .

The predicted oscillatory drop-off in the sedimentation coefficients of modeled arrays with increase in linker length is out-of-phase with measured values.

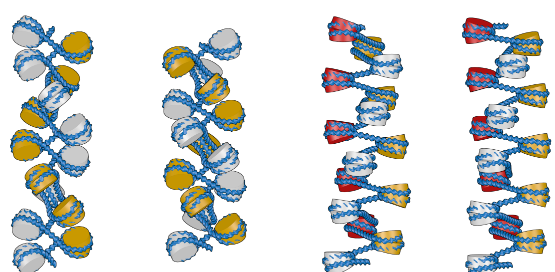


Correll et al (2012) Short nucleosome repeats impose rotational modulations on chromatin fibre folding EMBO J 31(10):2416–26.

Stefjord Todolli, unpublished data

Subtle differences in the nucleosome/linker template in known structures influence the global organization of and properties simulated arrays.

Changes in the nucleosome template convert a 2- to a 3-start structure with concomitant reorientation of nucleosomes relative to the global molecular axis.



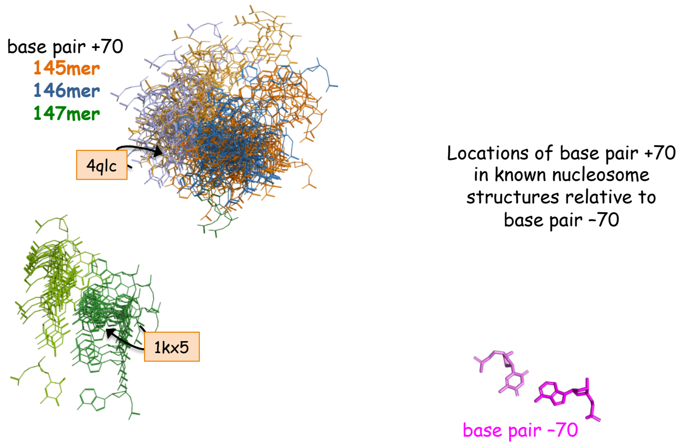
Linker	30-bp	28-bp	28-bp	30-bp
s_{12}	$43.2_{\pm1.7}$	$45.3_{\pm1.4}$	$45.8_{\pm1.6}$	$45.2_{\pm1.6}$
PDB template	4qlc	4qlc	1kx5	1kx5

unwrapped

Regular structures constructed from the mean rigid-body parameters between successive nucleosomes.

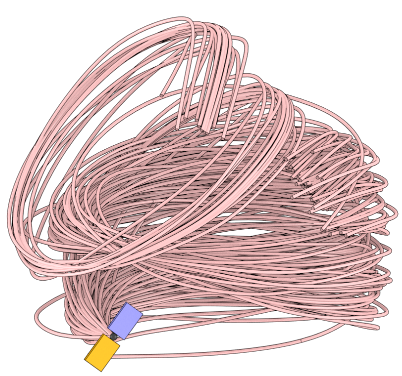
Stefjord Todolli, unpublished data

The placement of the DNA entering and exiting the nucleosome falls in distinct regions, with some sensitivity to the number of base pairs in known structures.



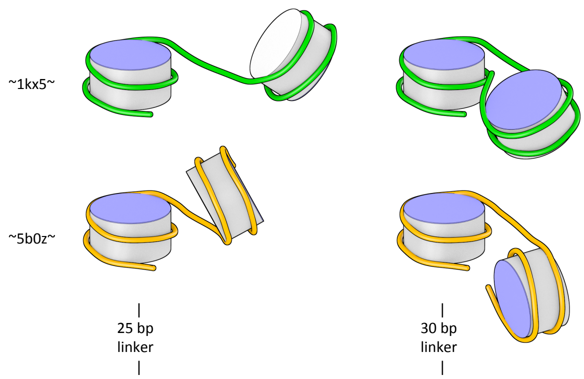
Stefjord Todolli, unpublished data

Nucleosome pathways in high-resolution structures fall into distinct groupings suggestive of motions of potential relevance to chromatin organization



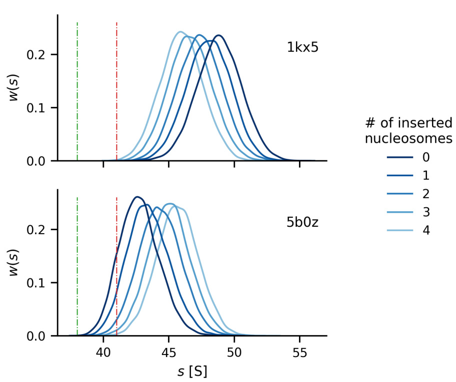
Stefjord Todolli, unpublished data

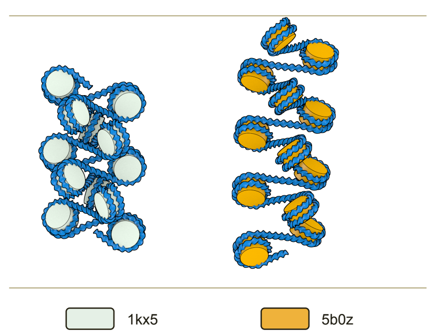
The differences in nucleosomal pathways lead to significant reorientation of successive nucleosomes and large-scale differences in simulated chromatin arrays.



Stefjord Todolli, unpublished data

The differences in nucleosomal pathways lead to significant reorientation of successive nucleosomes and large-scale differences in simulated chromatin arrays.





Stefjord Todolli, unpublished data

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