Structural DNA Nanotechnology

Three-Dimensional Self-Assembled Arrays:

Designed Crystals.

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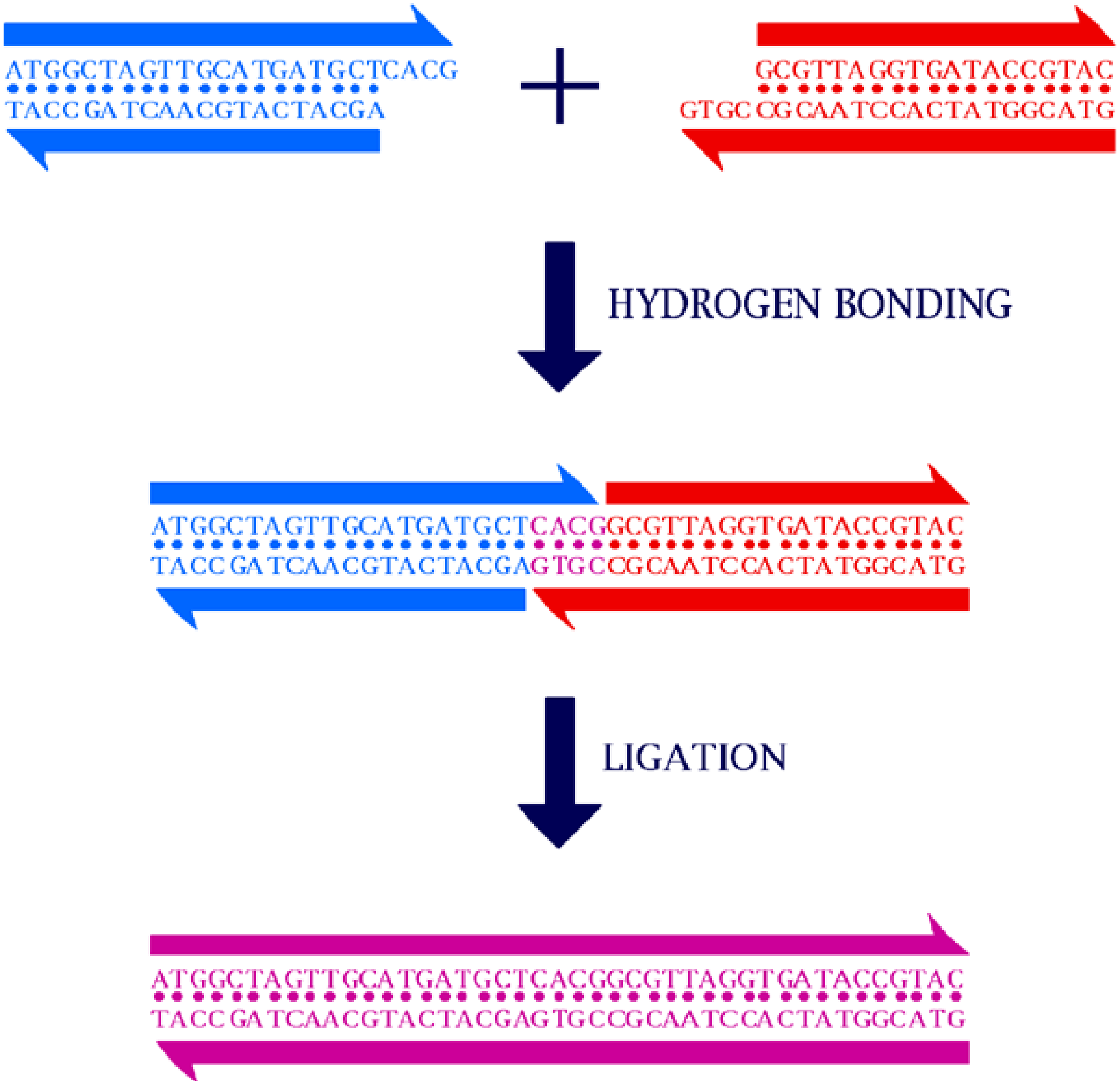
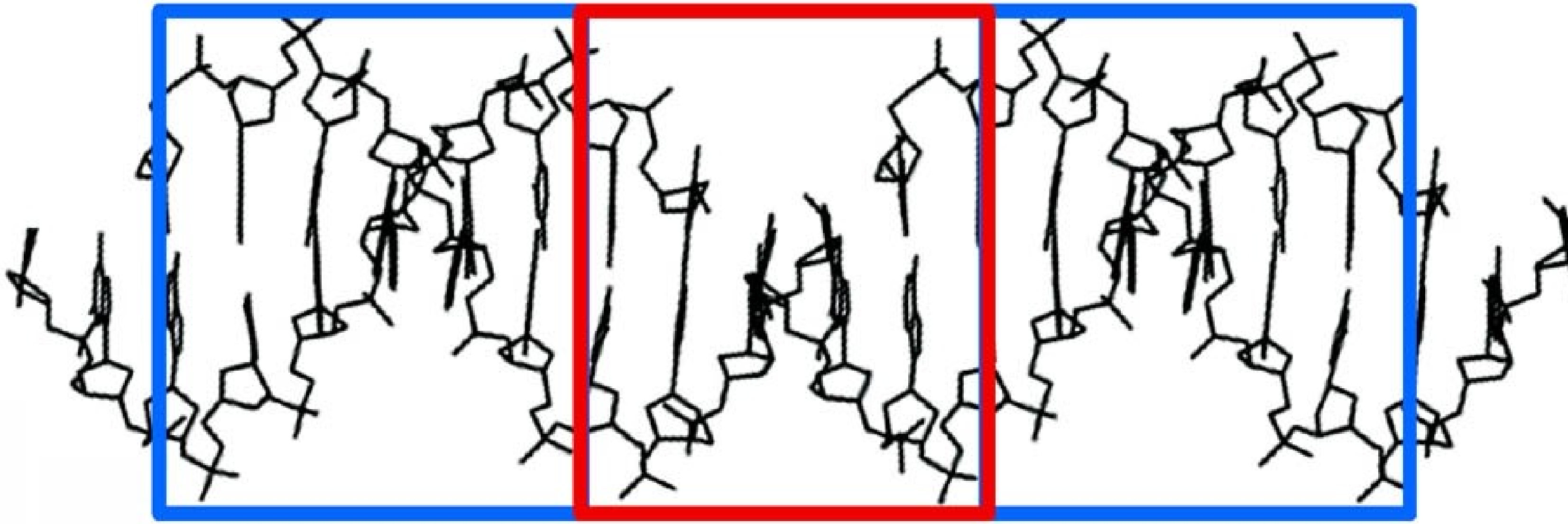
Sticky-Ended Cohesion: Smart Affinity



Sticky-Ended Cohesion: Structure



Qiu, H., Dewan, J.C. & Seeman, N.C. (1997) *J. Mol. Biol.* **267**, 881-898.

Holliday cross-over junctions

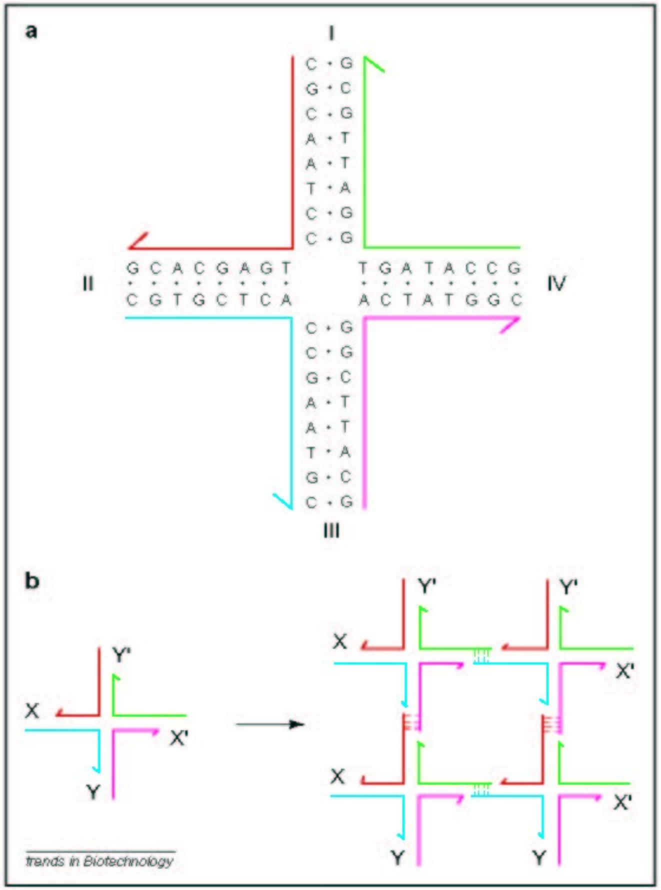
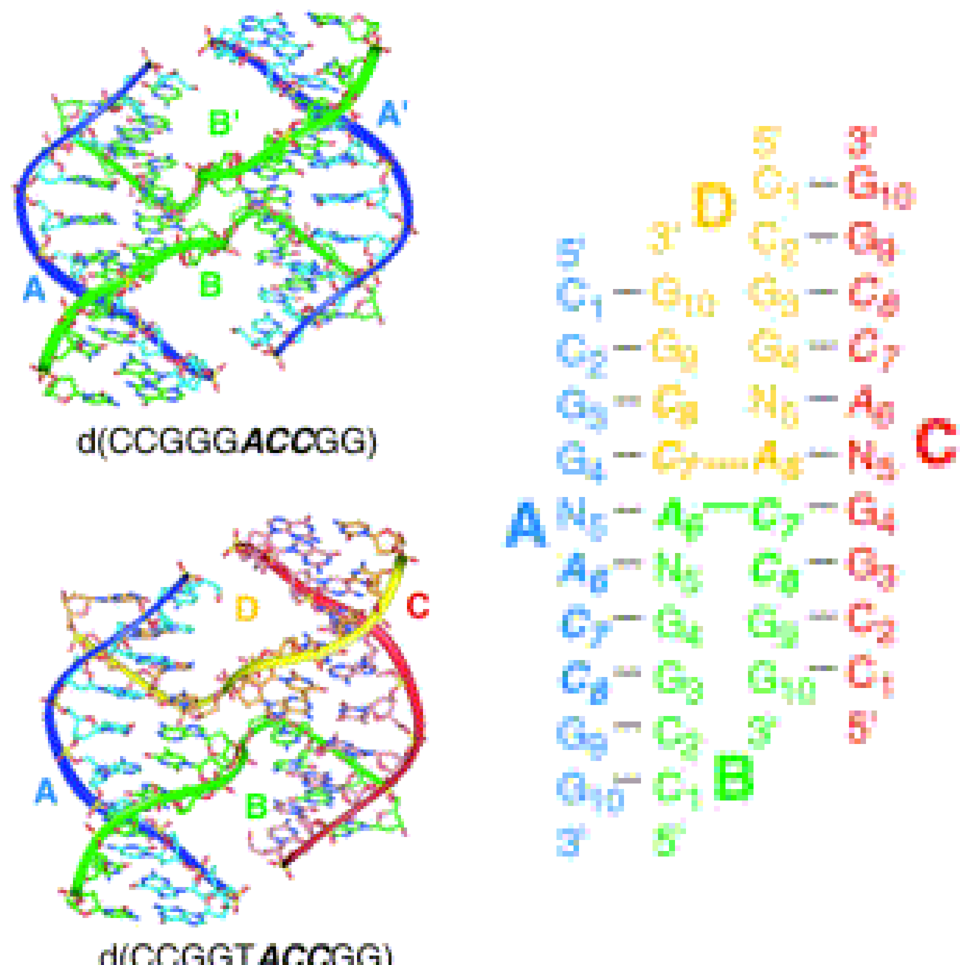


Figure 1

(**a**) A branched DNA molecule with four arms. The four strands, here identified by color, combine to produce four arms, labeled with Roman numerals. The branch point of this molecule is fixed. (**b**) The formation of a two-dimensional lattice from a four-arm junction with sticky ends. X and Y are sticky ends, and X′ and Y′ are their complements. Four of the monomeric junctions on the left are complexed in parallel orientation to yield the structure on the right. DNA ligase can close the gaps left in the complex. The complex has maintained open valences, so that it could be extended by the addition of more monomers. A DNA double helix is about 200 nm wide and its helical repeat is 10–10.6 bp, which produces a pitch of 340–360 nm. Thus, constructions made from DNA will have features on the nanometer scale.

(b) ACC trinucleotide junctions



OBJECTIVES AND APPLICATIONS FOR OUR LABORATORY

ARCHITECTURAL CONTROL AND SCAFFOLDING

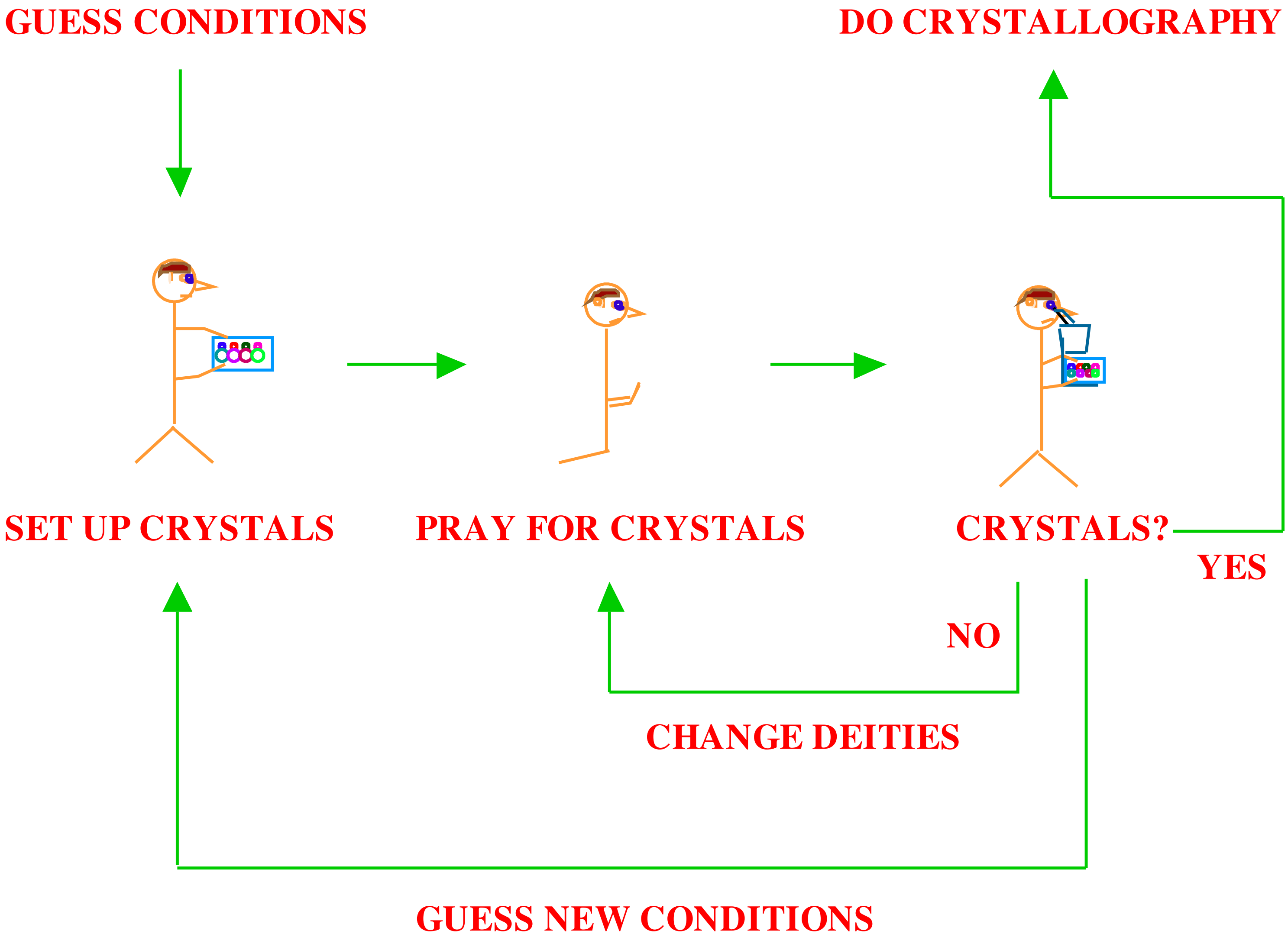
➡ [1] MACROMOLECULAR CRYSTALLIZATION (PERIODIC IN 2D AND 3D).
[2] NANOELECTRONICS ORGANIZATION (PERIODIC IN 2D AND 3D).
[3] DNA-BASED COMPUTATION (APERIODIC IN 2D OR 3D).
[4] CONTROL OF POLYMER AND MATERIALS COMPOSITION & TOPOLOGY.

NANOMECHANICAL DEVICES

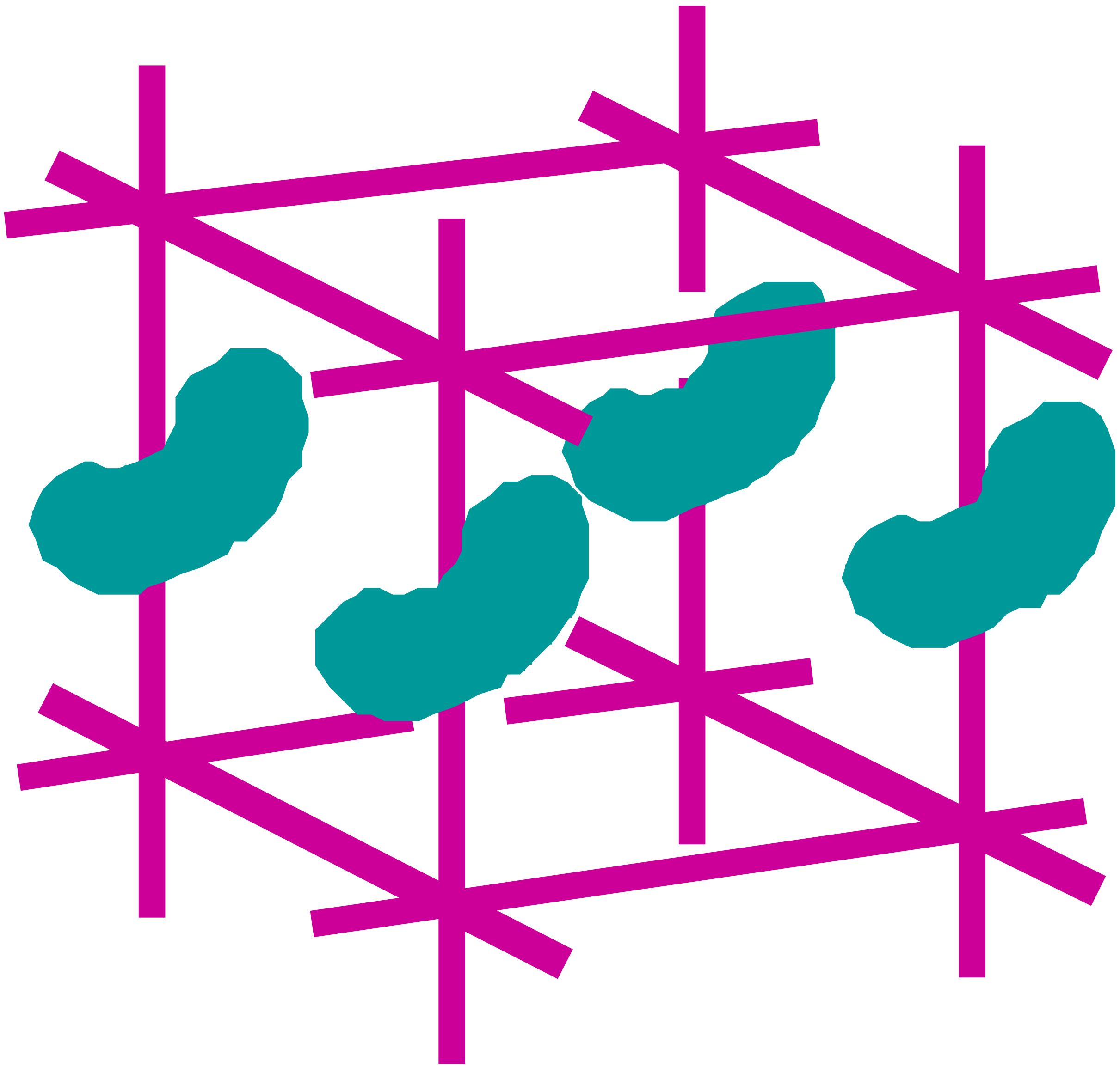
[1] NANOROBOTICS.
[2] NANOFABRICATION.

SELF-REPLICABLE SYSTEMS

CURRENT CRYSTALLIZATION PROTOCOL

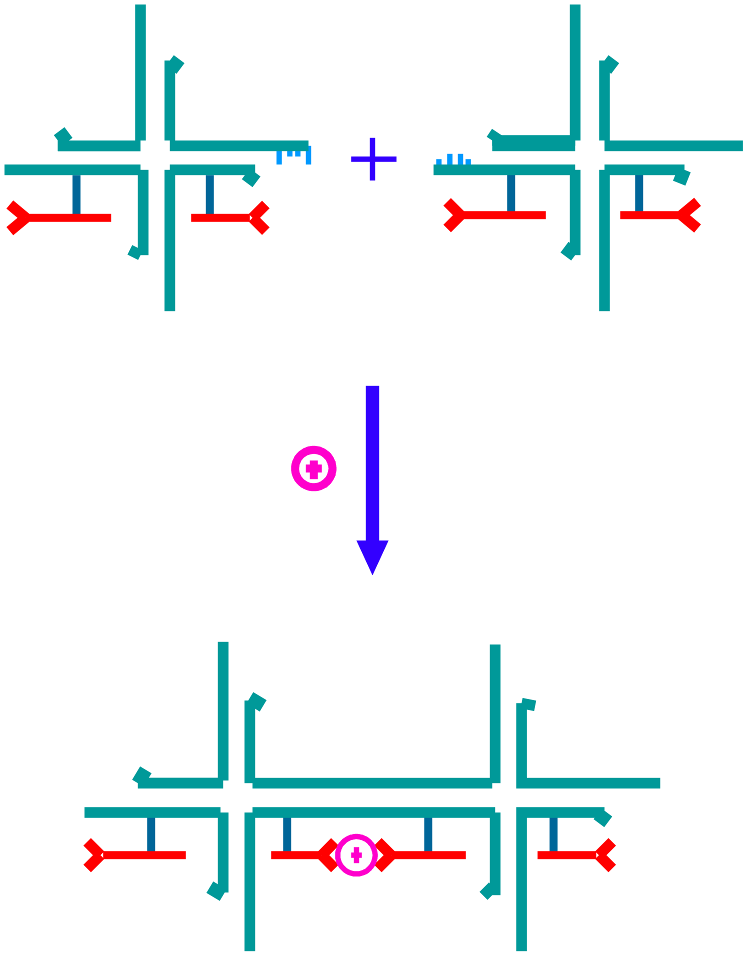


A New Suggestion for Producing Macromolecular Crystals



Seeman, N.C. (1982), *J. Theor.Biol.* **99**, 237-247.

A Method for Organizing Nano-Electronic Components

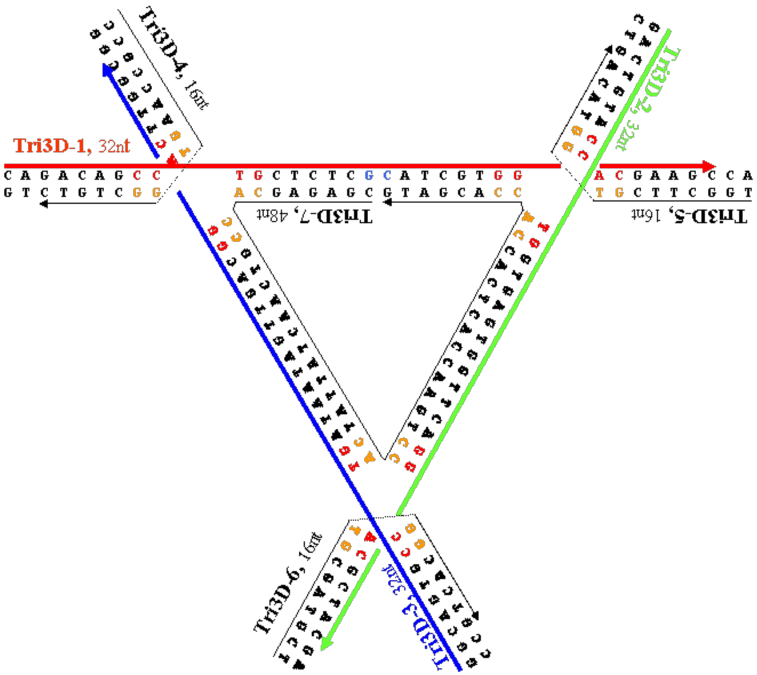


Robinson, B.H. & Seeman, N.C. (1987), *Protein Eng*. **1**, 295-300..

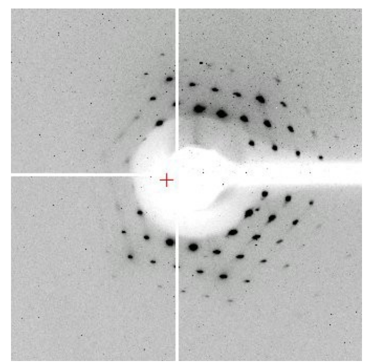
Construction of Crystalline Arrays

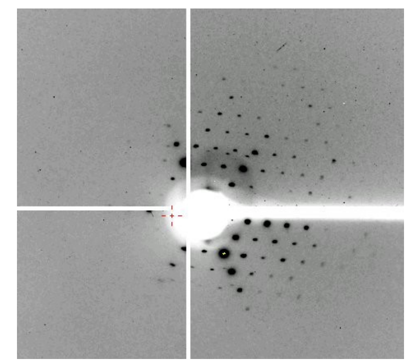
A 3D DNA Tensegrity Triangle

[D.Liu, M. Wang, Z. Deng, R. Walulu & C.Mao, *J. Am. Chem. Soc.* **126**, 2324-2325 (2004)]



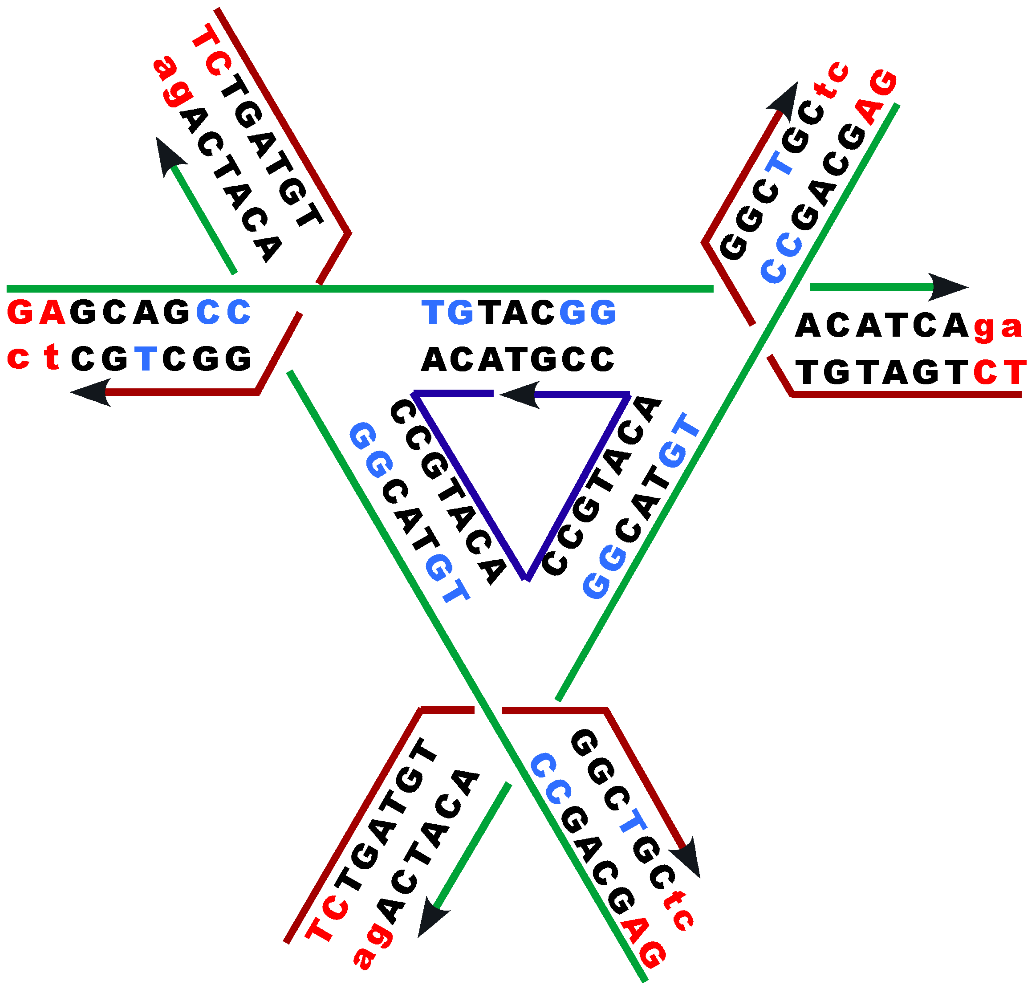
X-Ray Diffraction:
Predicted Spacings and
Rhombohedral Symmetry
Resolution: ~10Å





Designed 142 A Edges

A Small Threefold Pseudosymmetric DNA Tensegrity Triangle



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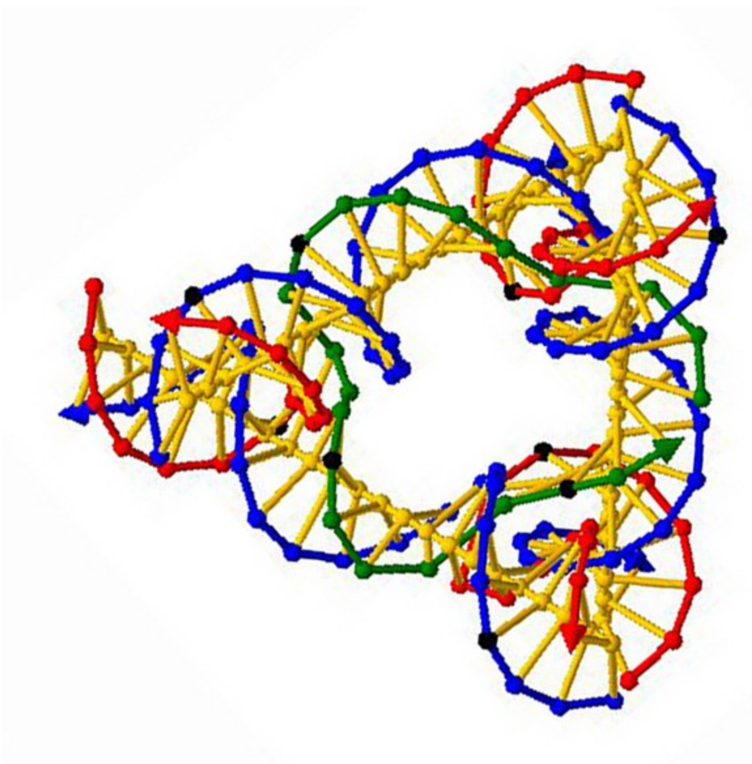
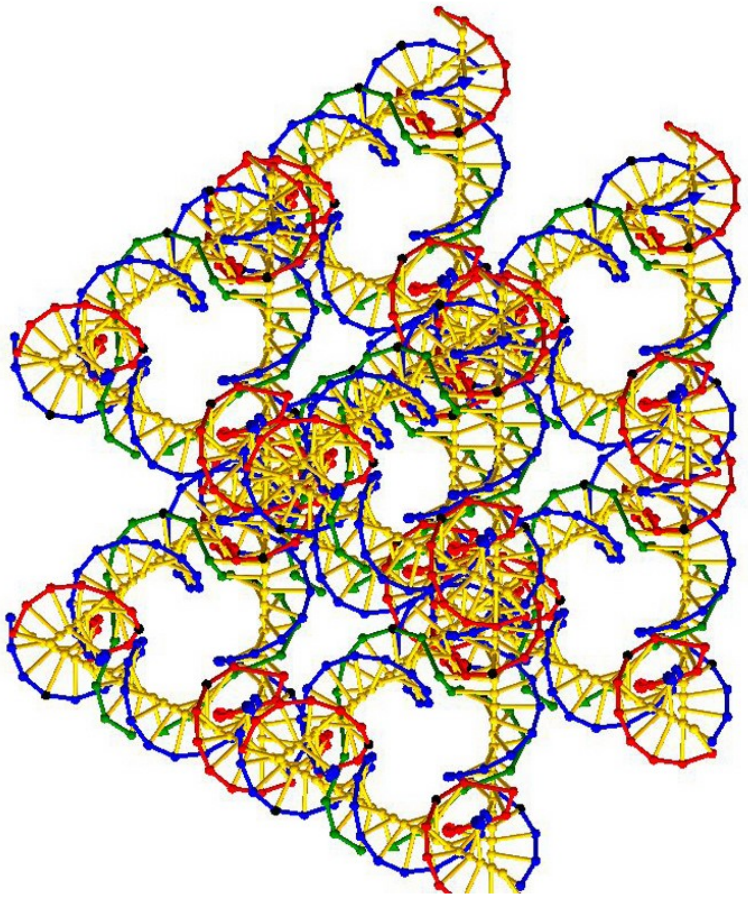
Triangle Schematics

Individual Tile



3D Array



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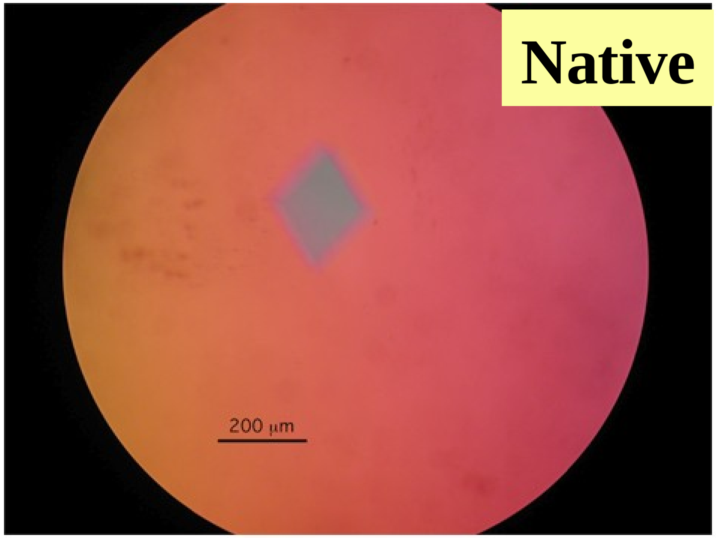
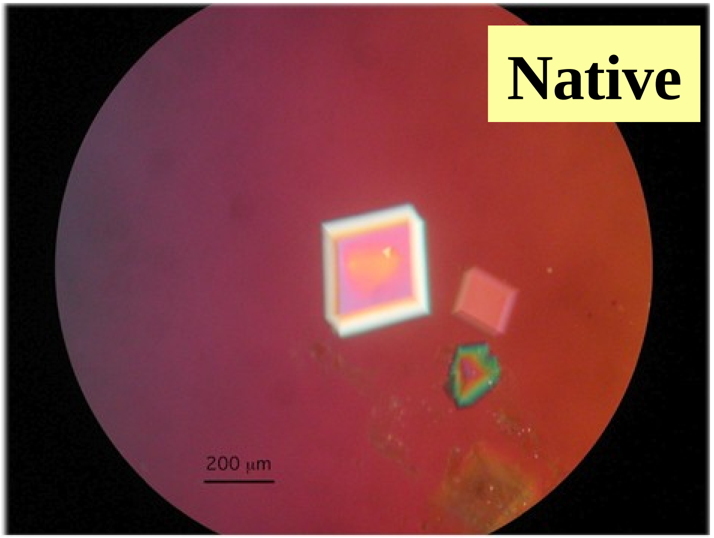
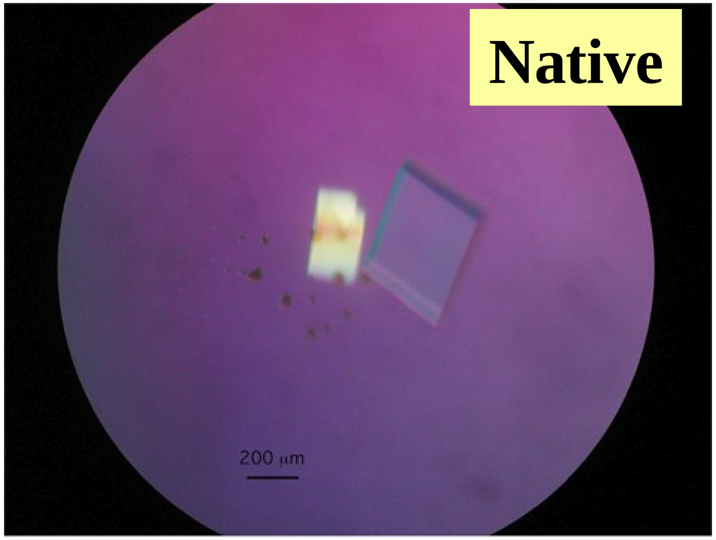
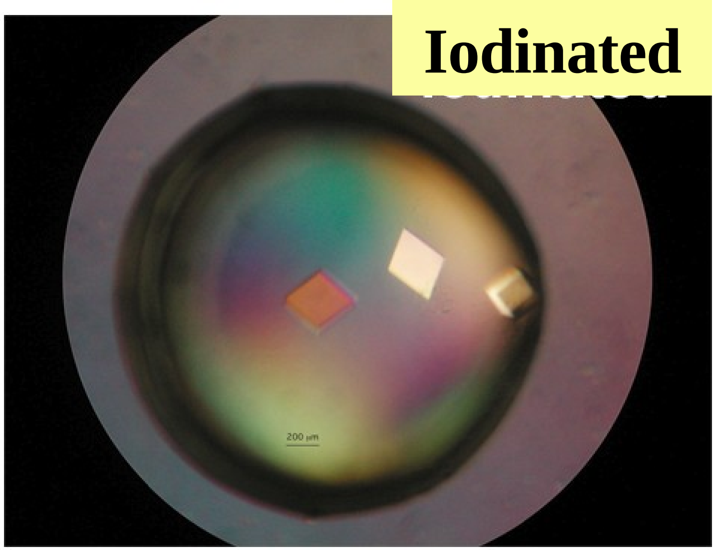
Crystal Images









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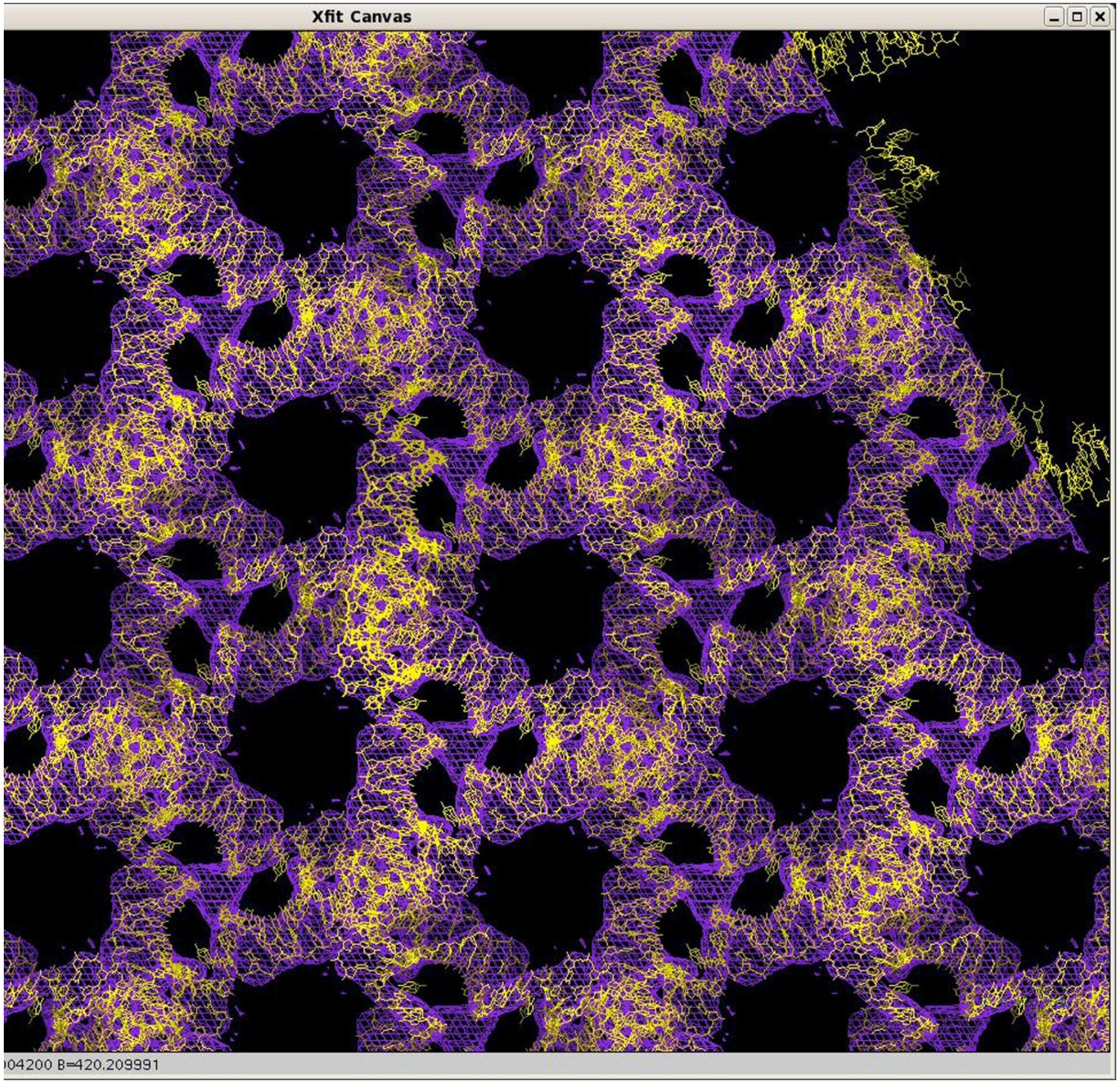
View down the 3-Fold Axis
5 Å Electron Density map

Electron Density calculated via SAD phasing using 4 iodines per 42 NA's



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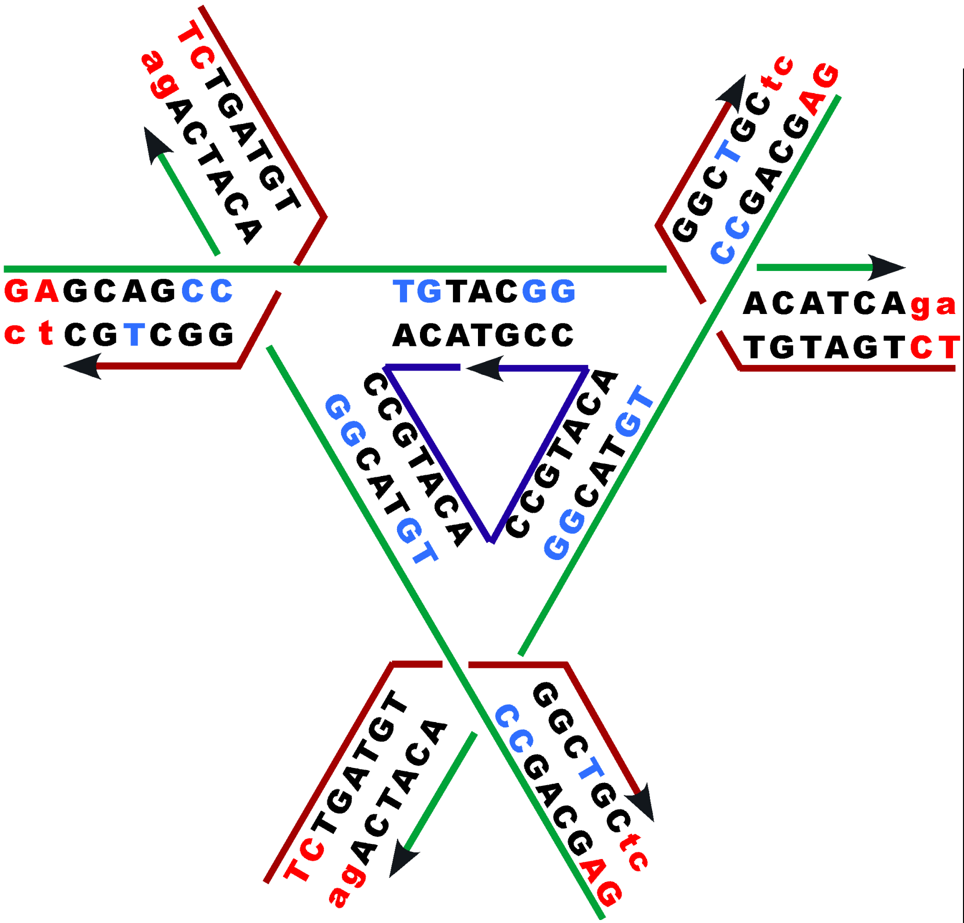
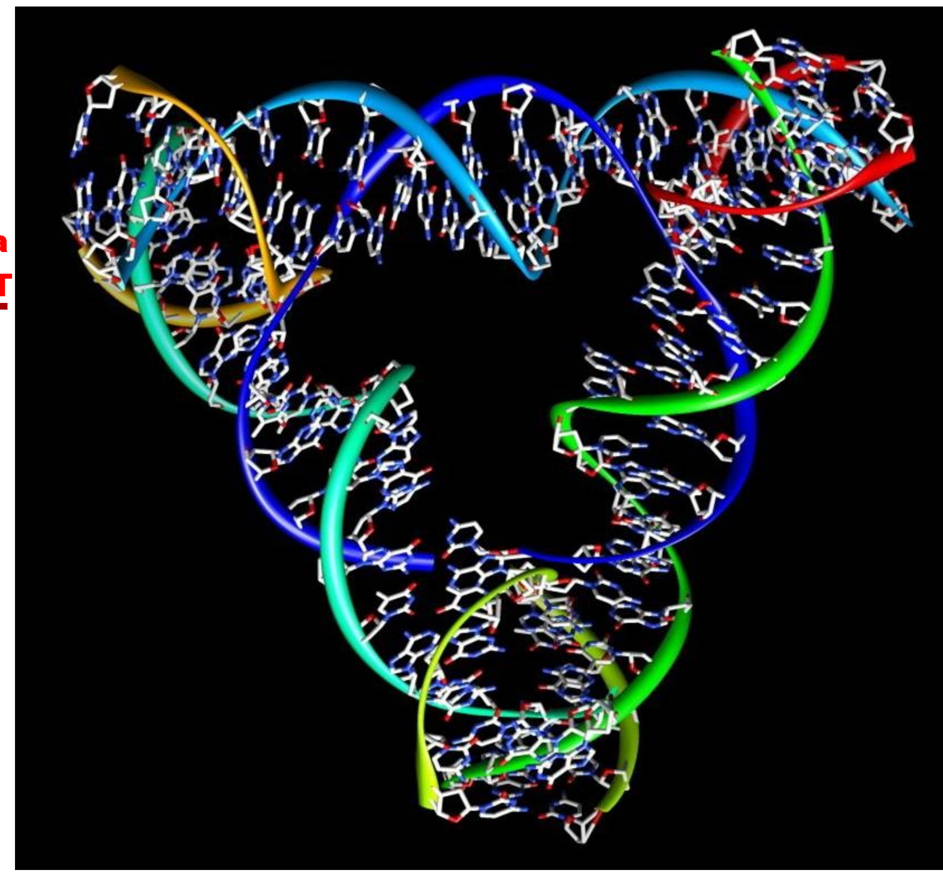
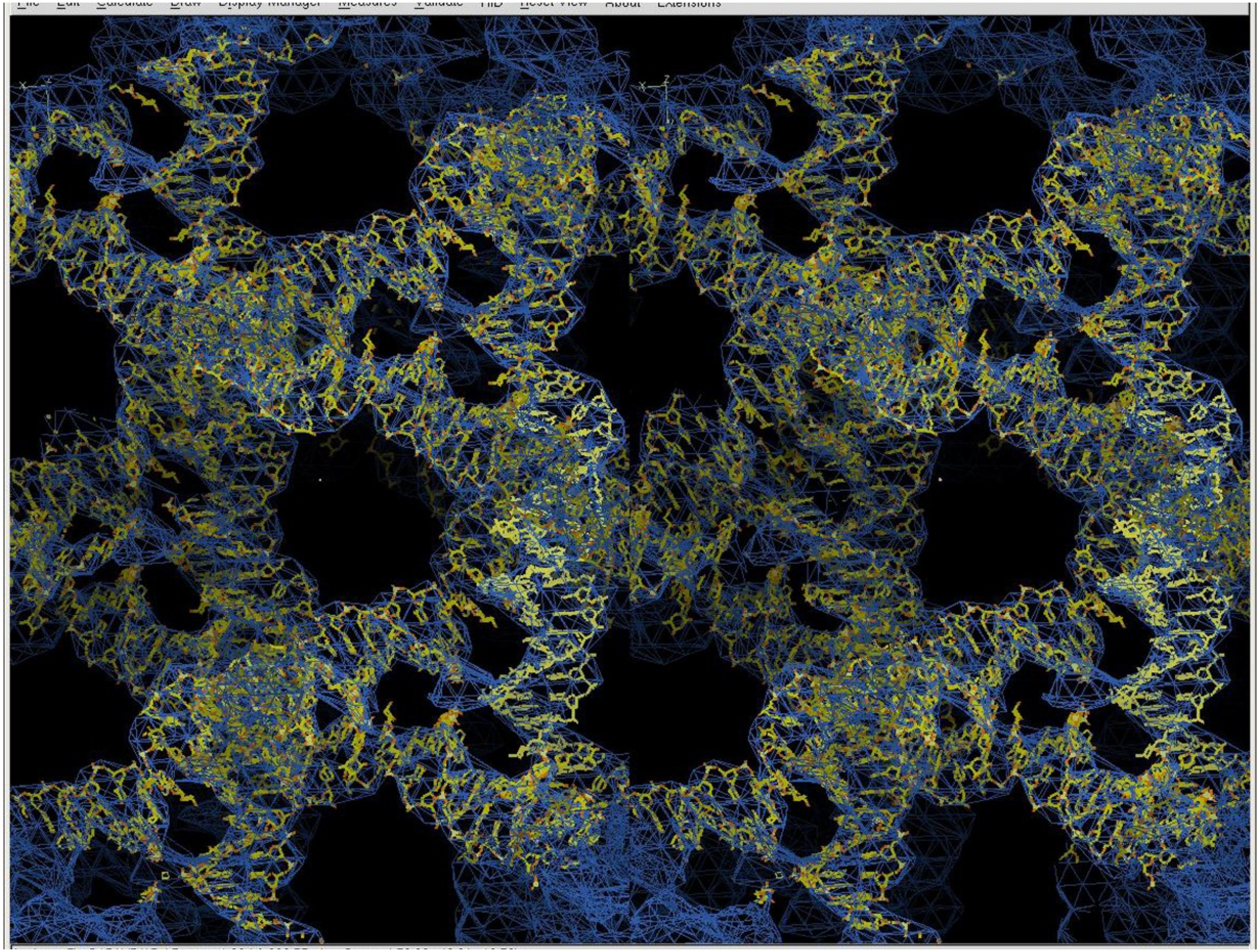
21 NA Edge Triangle: Schematic & Ribbon 3D model





Crude 5 Å Fit in Stereo



R3; **a** = 68.28; α = 102.44°

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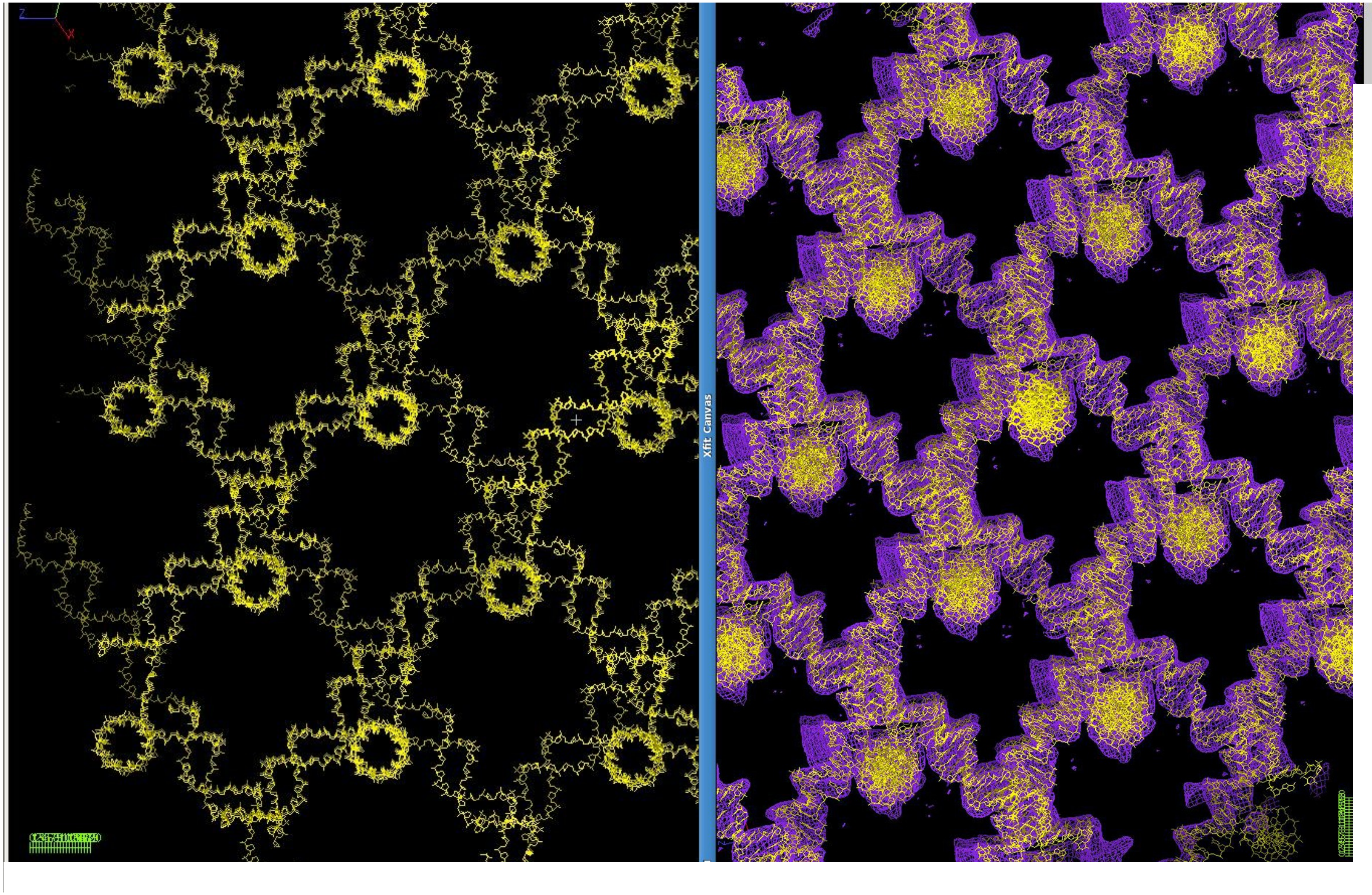
View Down a Helix Axis
Electron Density from SAD-phased (Iodine) Map



This is B-DNA

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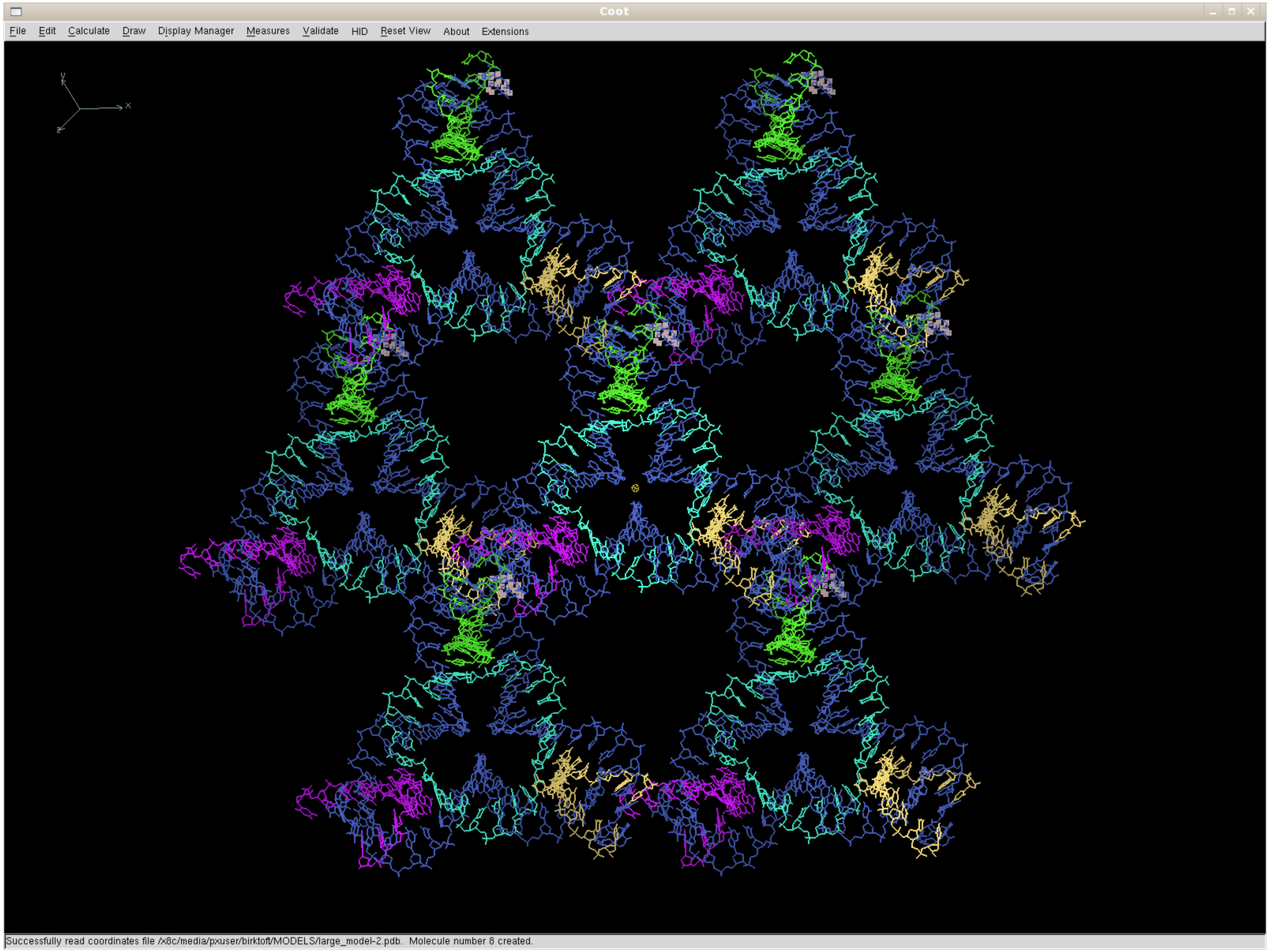
Environment of a Single Triangle



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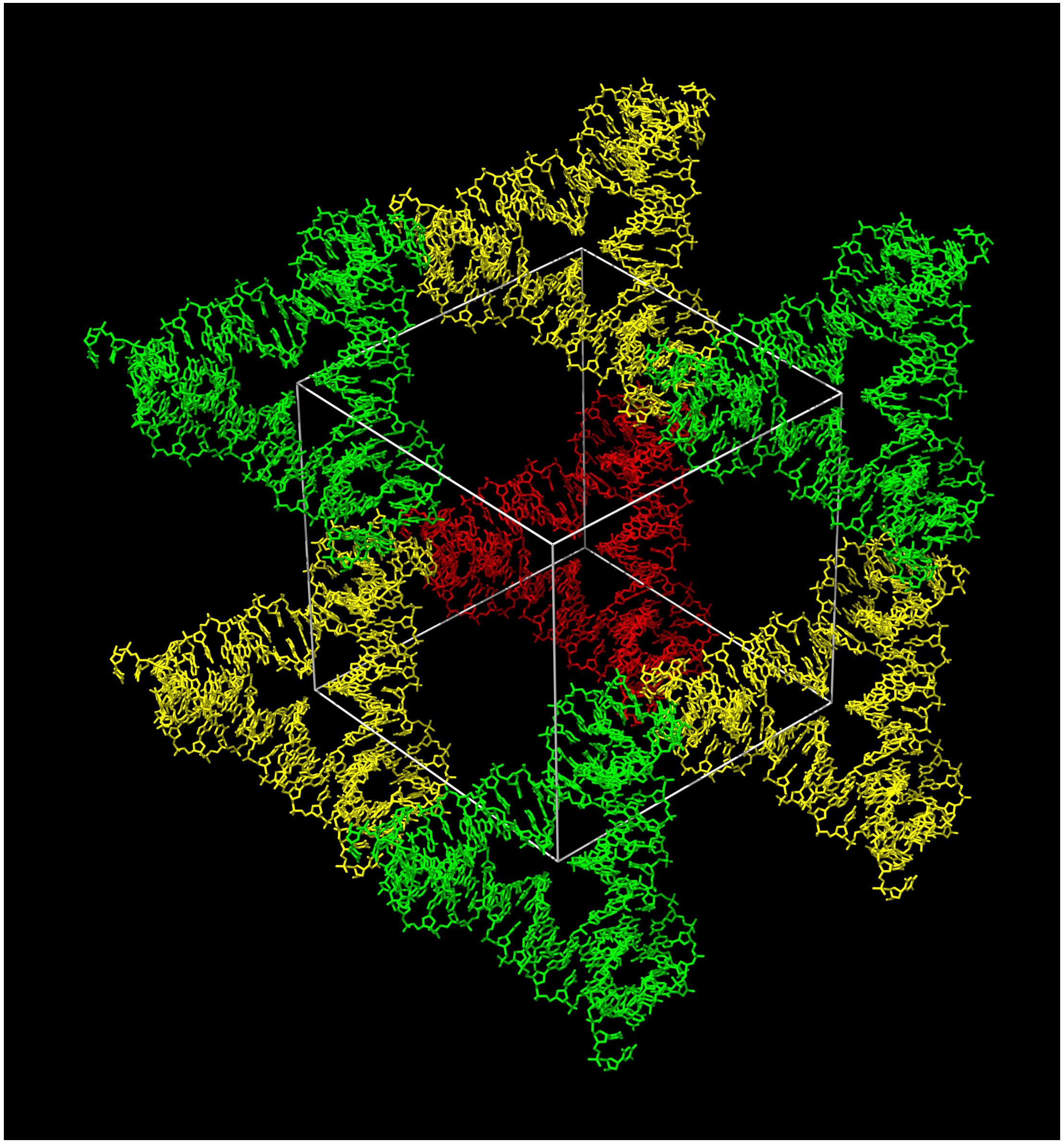
The Rhombohedral Cavity



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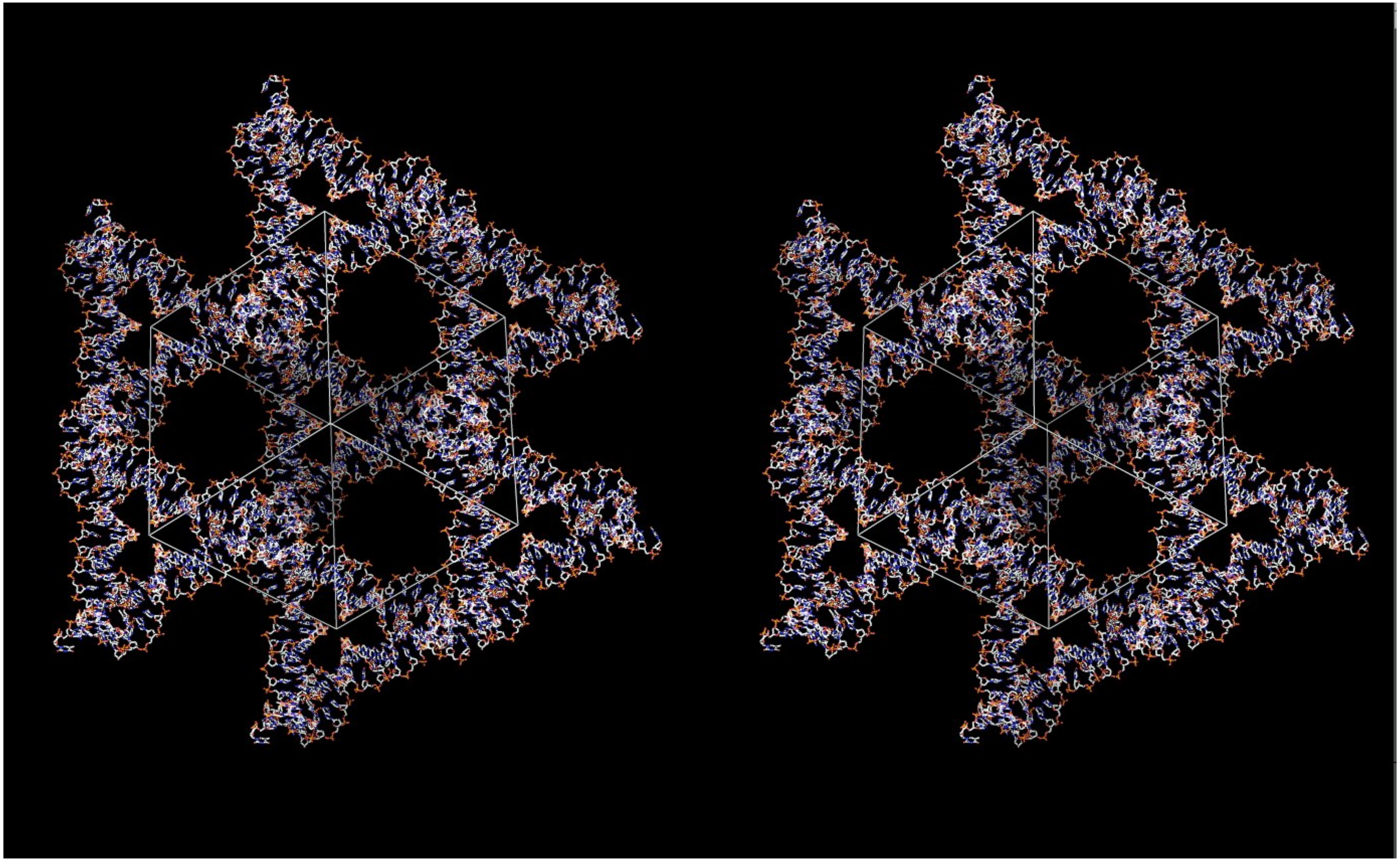
Stereo View of the Rhombohedron



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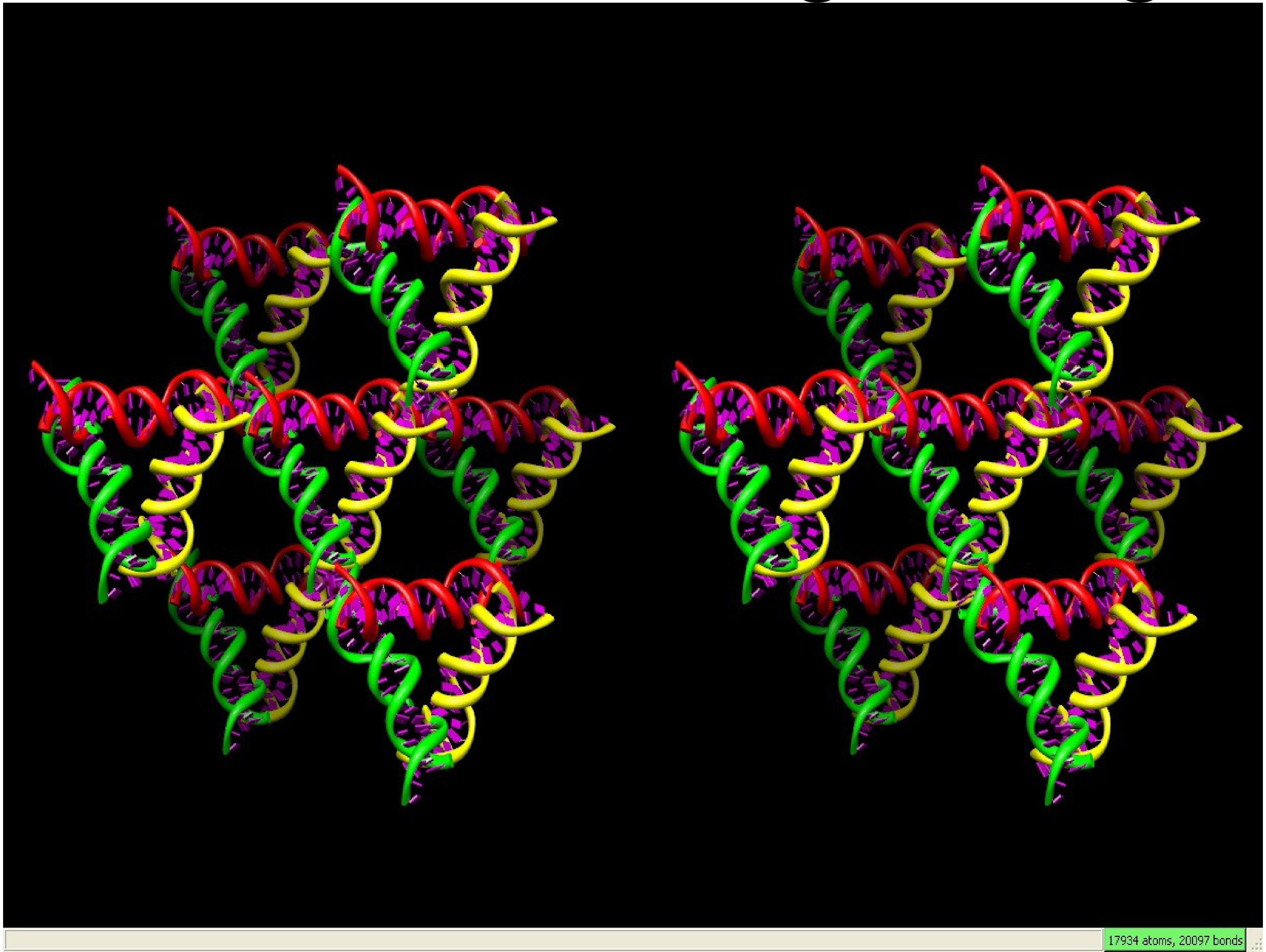
Environment of a Single Triangle



A Four-Turn Triangle Designed Lattice

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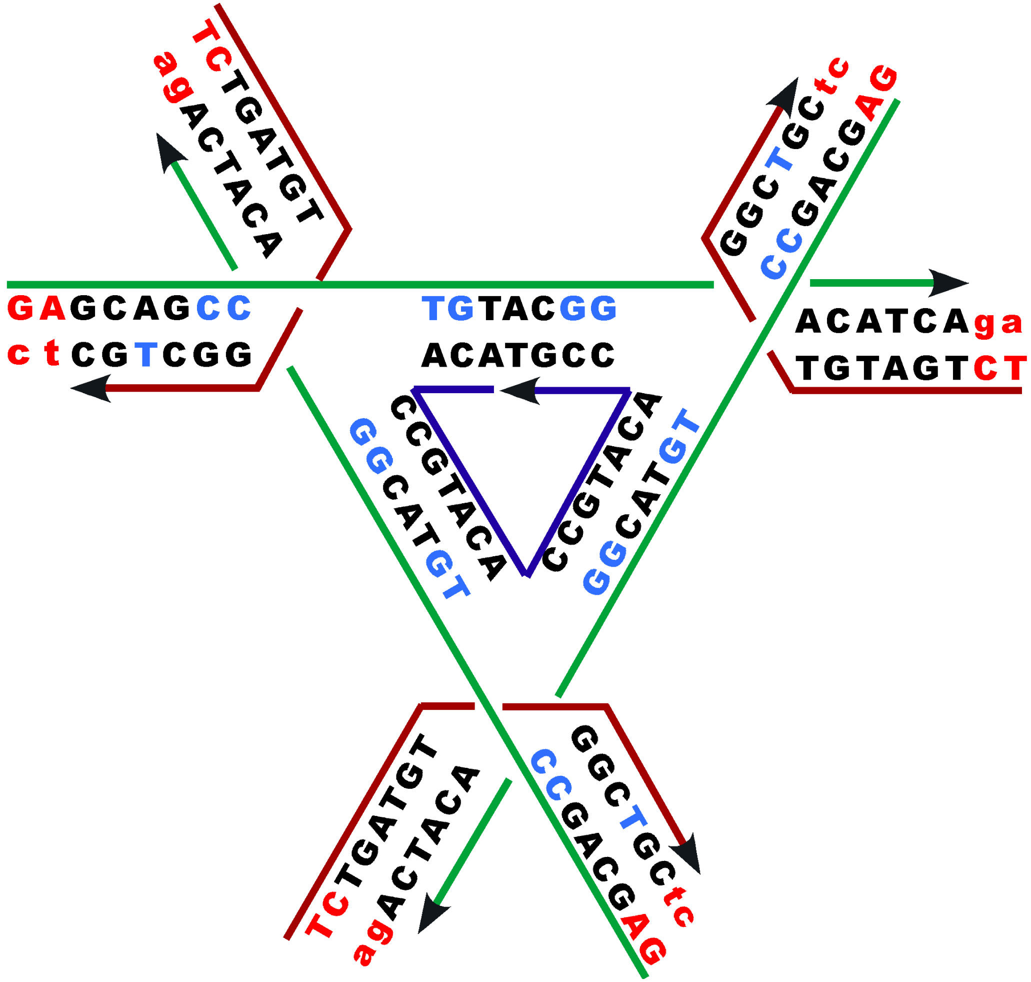
Jens Birktoft; Ruojie Sha,
Chengde Mao (Purdue)

A Small Threefold Pseudosymmetric DNA Tensegrity Triangle



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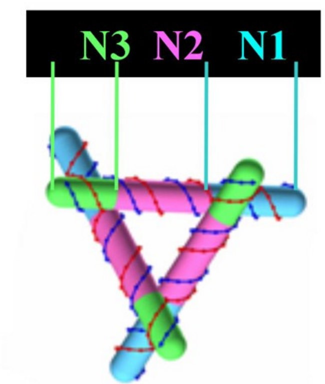
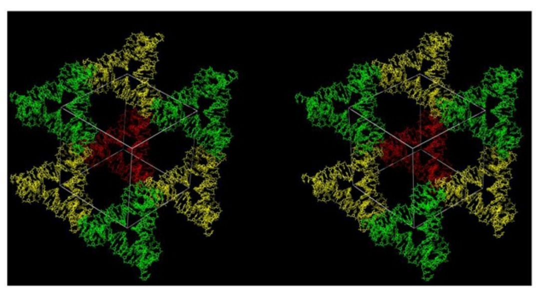
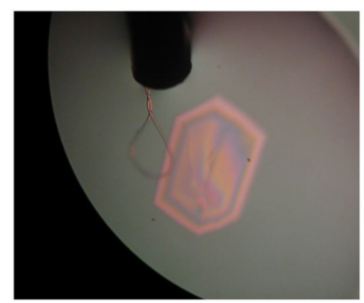
Summary of Results with Triangle Crystals

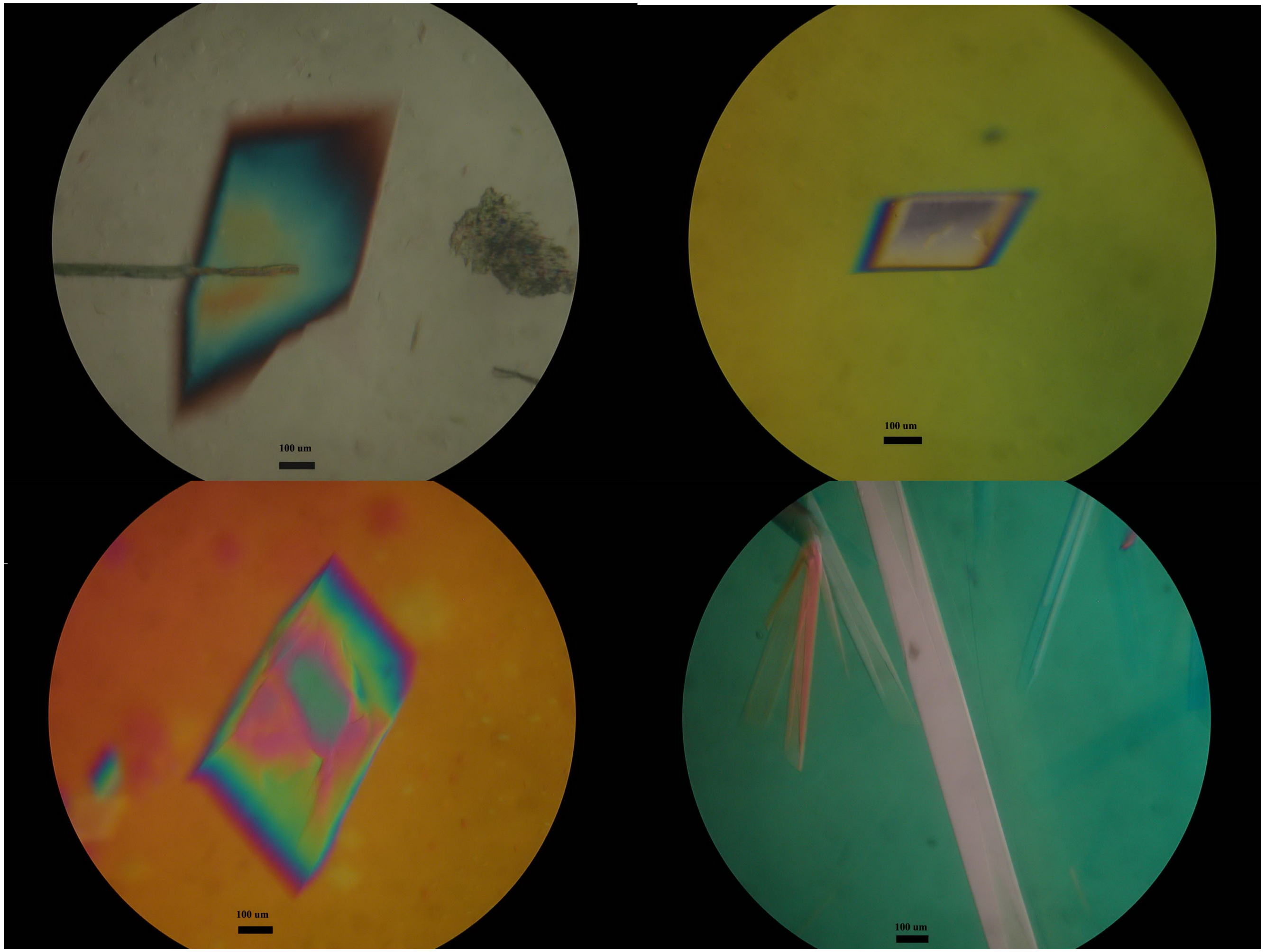
	Symmetry	Unit Length (base)	Length between Crossovers (base)	Cell Dimensions (in R_3)	Resolution (Å)	Cross Sectional Size($\AA^2$_10^3)	Cavity Size ($\AA^3$_10^5)
1	+	21	7	a = 68.3, α =102.4	4.0	1.9	1.0
2	-	21	7	a = 68.0, α = 102.6	5.0	2.6*	1.3*
3	+	**31**	17	a = 102.0, α = 112.7	6.1	6.8*	5.2*
4	-	**31**	17	a = 100.9, α = 111.6	6.3	6.8*	5.2*
5	+	32	18	a = 103.6, α = 113.6	6.5	7.2*	5.6*
6	-	32	18	a = 103.3, α = 112.2	6.5	7.2*	5.6*
7	+	**42**	17	a= 135.1, α = 111.2	11.0	14.0*	15.4*
8	+	**42**	28	a = 134.9, α = 117.3	8.0	14.0*	15.4*







Crystals of Triangles with 42-Nucleotide-Pair Edges Triangles



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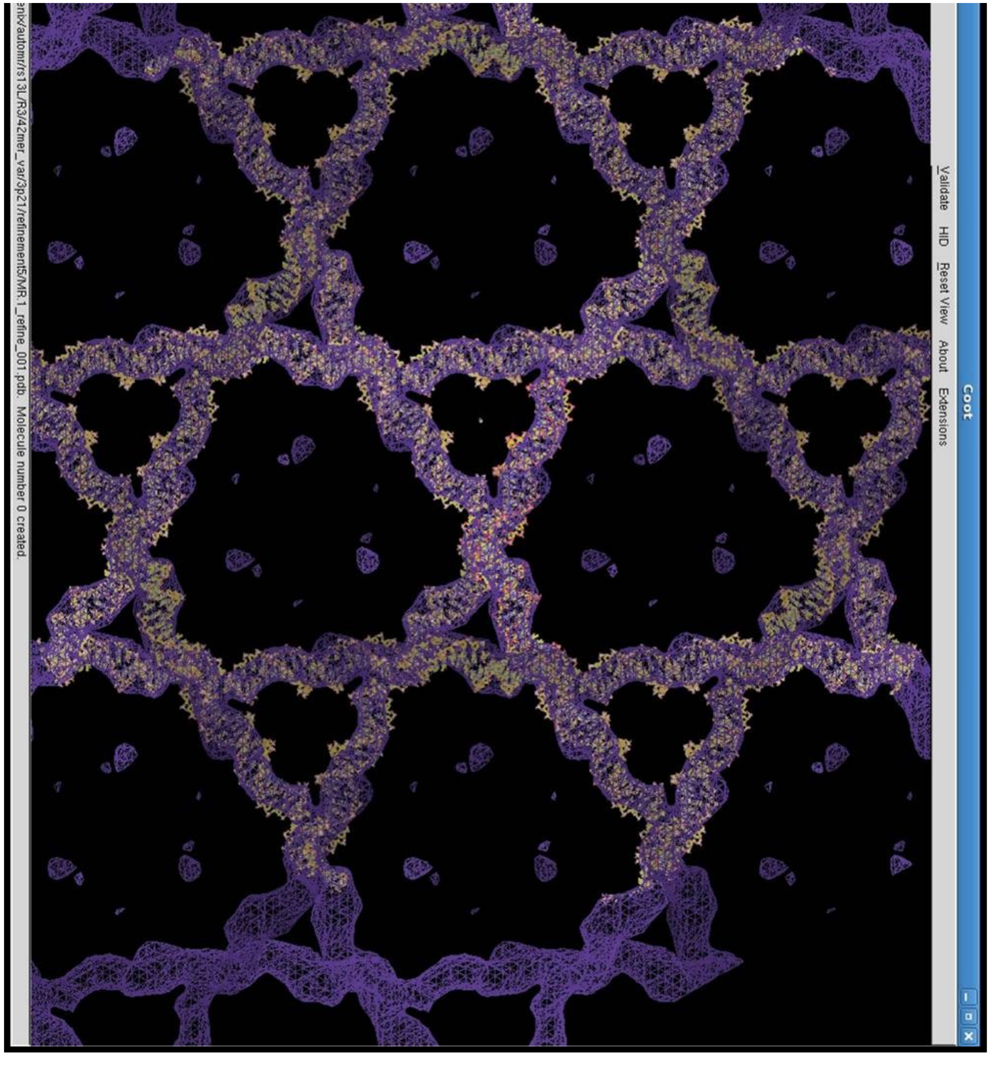
Summary of results with Triangle Crystals

Symmetry	Edge Length (bases)	Length between Crossovers	Rhombohedral Cell Dimensions	Resolution (Å)	Cross Section (nm^2)	Cavity Size (nm^3)
+	21	7	a= 68.3 Å, α=102.4°	4.0	23	103
-	21	7	a= 68.0 Å, α=102.6°	5.0	23	101
+	31	17	a=102.0 Å, α=112.7°	6.1	62	366
-	31	17	a=100.9 Å, α=111.6°	6.3	61	373
+	32	18	a=103.6 Å, α=113.6°	6.5	64	367
-	32	18	a=103.3 Å, α=112.2°	6.5	64	395
+	42	17	a=135.1 Å, α=110.9°	11.0	123	1104
-	42	17	a=133.7 Å, α=111.3°	14.0	120	1048
+	42	28	a=134.9 Å, α=117.3°	10.0	117	643

‘Symmetry’ refers to deliberate 3-fold disorder.
Edge lengths and inter-junction distances (within triangles) are given in nucleotide pairs
The cross-sectional area and cavity size are derived from the crystal structures. Cross-sections and cavity sizes are estimated by subtracting two radii of the double helix (~10 Å) from the unit cell dimensions.

3-Fold Axis Projection of a Triangle with 42-Nucleotide-Pair Edges at 11 Å

Diffraction data collected at NSLS beam lines X6A & X25.
Solved via MR using fragments of B-DNA.
After rigid–body refinement R-factor ~ 35%/38%.



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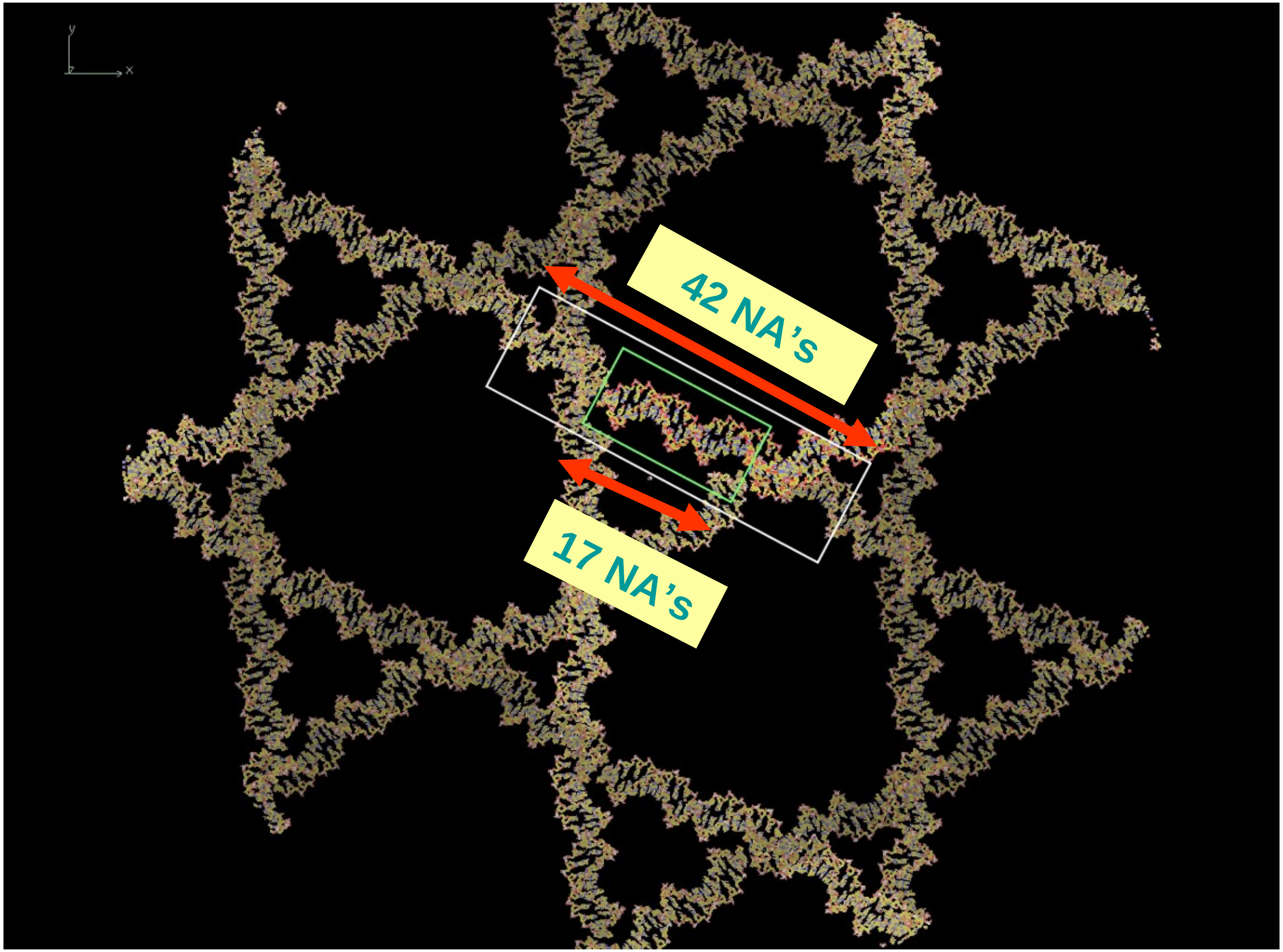
Clarification of Components



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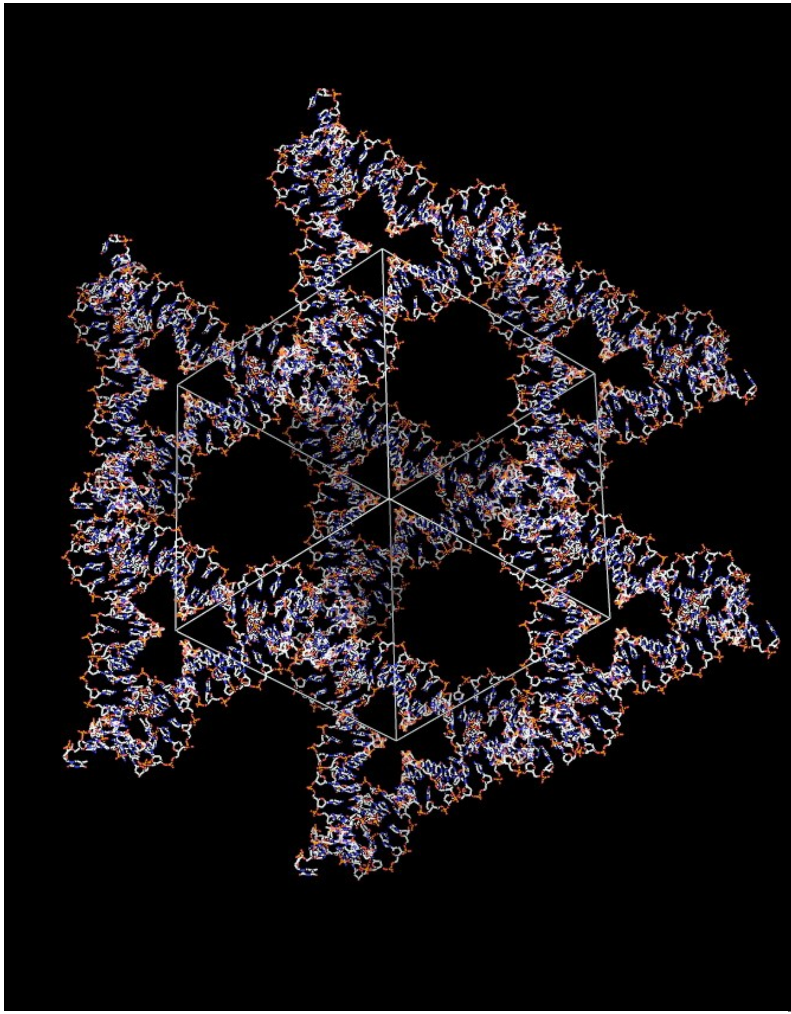
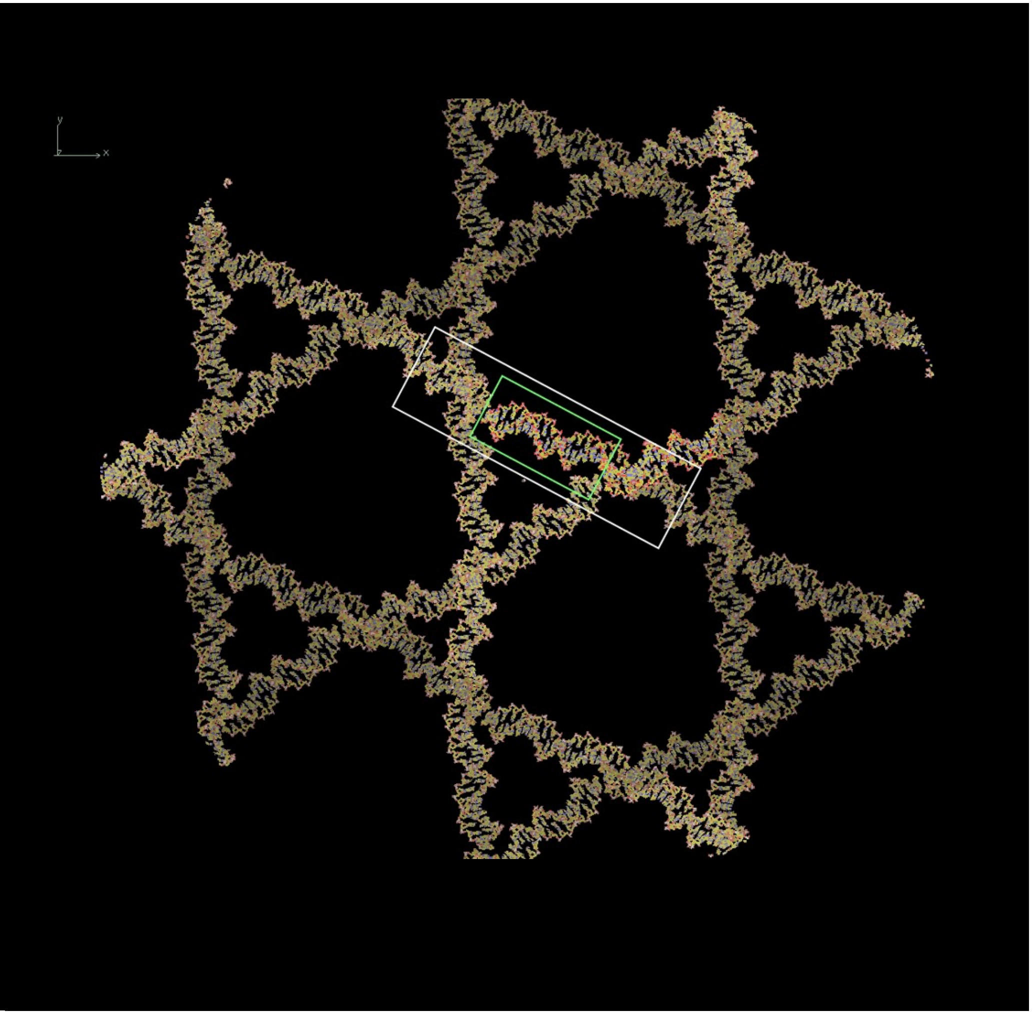
21 & 42 NA's Edge Rhombohedron





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Summary of results with Triangle Crystals

Edge Length	Symm.	Inter juncti	R3 Cell Dimentsions	Volume (nm^3)	H3 Cell Dimensions	Volume (nm^3)	Resol.	Cross Section (nm^2)	Cavity Size (nm^3)
21	+	7	a= 68.3 Å α=102.4°	292336	a=b= 106.5, c= 89.4°	877009	4.0 Å	23	103
21	-	7	a= 68.0 Å α=102.6°	287577	a=b= 106.1, c= 88.4	862731	5.0 Å	23	101
31	+	17	a=102.0 Å α=112.7°	702555	a=b= 169.8, c= 84.4	2107666	6.1 Å	62	366
31	-	17	a=100.9 Å α=111.6°	721765	a=b= 166.9, c= 89.8	2165296	6.3 Å	61	373
32	+	18	a=103.6 Å α=113.6°	695139	a=b= 173.4, c= 80.1	2085415	6.5 Å	64	367
32	-	18	a=103.3 Å α=112.2°	750720	a=b= 171.5, c= 88.4	2252161	6.5 Å	64	395
42	+	17	a=135.1 Å α=110.9°	1790781	a=b= 222.51, c= 125.3	5372343	11.0 Å	123	1104
42	-	17	a=133.7 Å α=111.3°	1703911	a=b= 220.8, c= 121.1	5111732	14.0 Å	120	1048
42	+	28	A=134.9 Å, α=117.3°	1029774	a=b= 230.4, c= 67.2	3089321	10.0 Å	117	643