

Model-building of helices into electron-density maps

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Rapid building of models for regions containing regular secondary-structure

Helices:

Identification: rods of density at low resolution

Strands:

Identification: β structure as nearly-parallel pairs of tubes

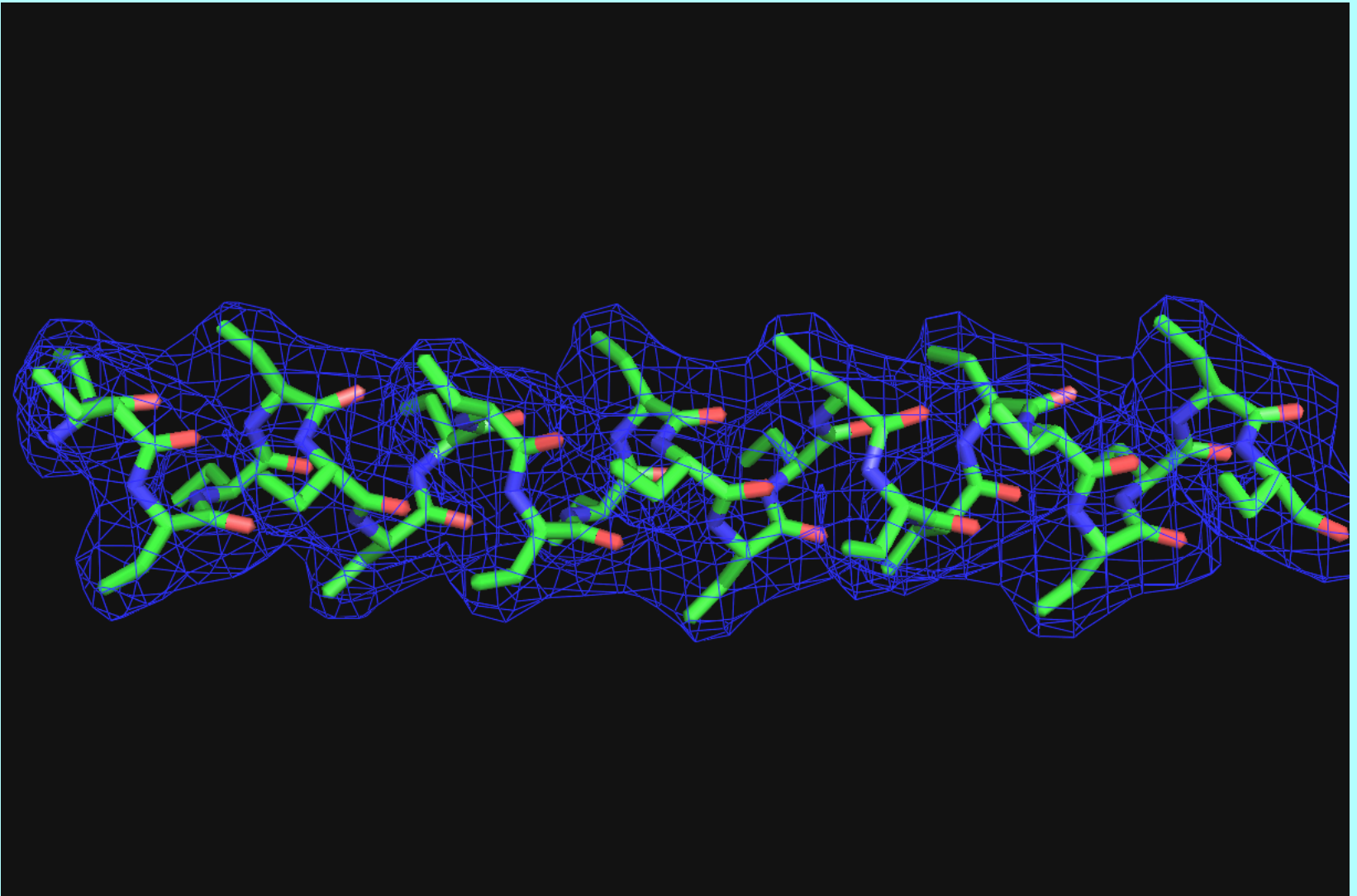
Any protein chains (trace_chain):

Identification: $C\alpha$ positions consistent with density and geometry of protein chains

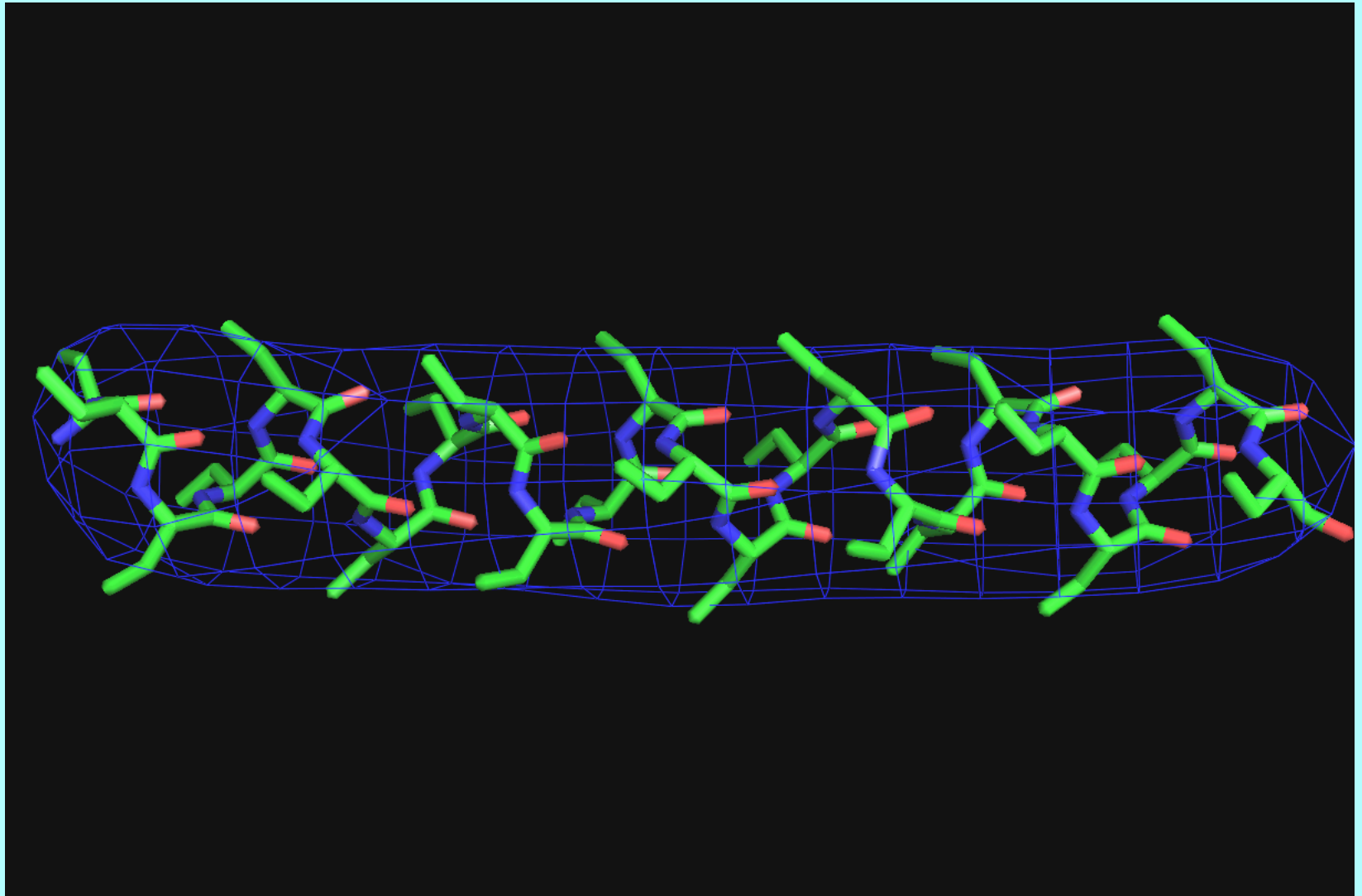
RNA/DNA:

Identification: match of density to averaged A or B-form template

Model α -helix; 3 Å map

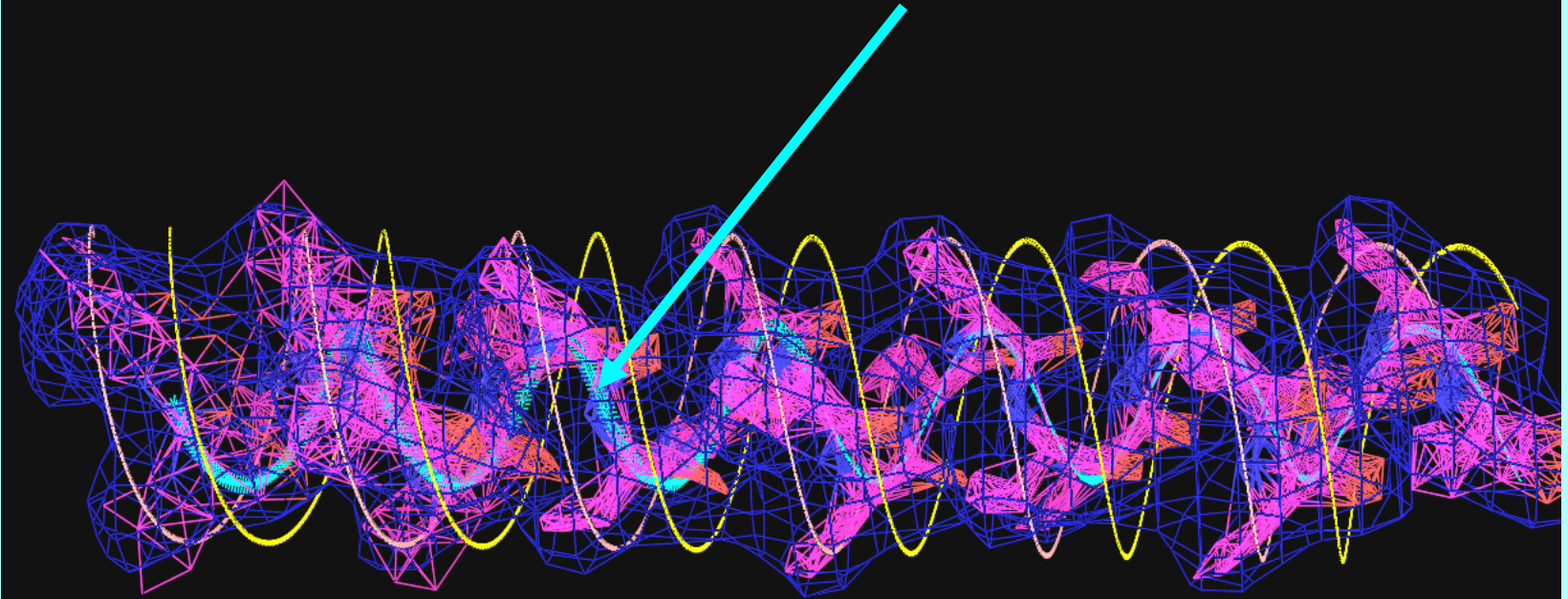


Model α -helix; 7 Å map



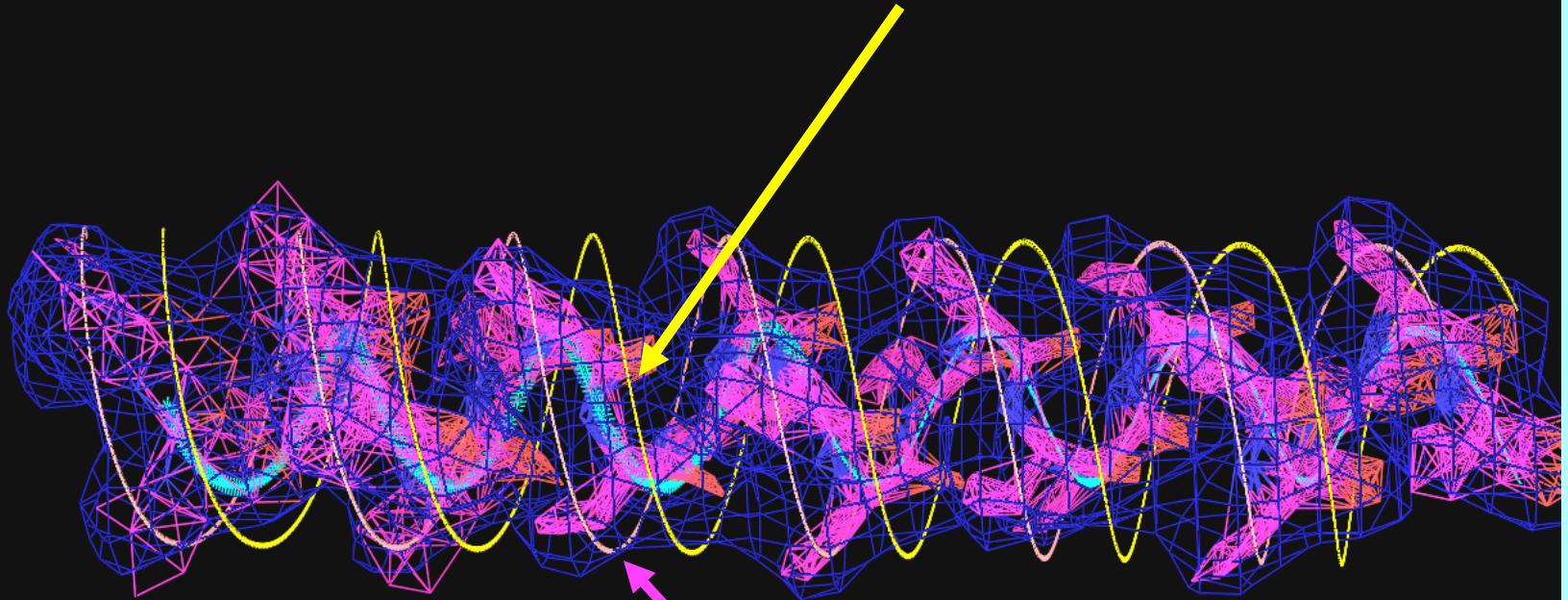
Trace main-chain with ideal helix, allowing curvature

2 Å radius, 5.4 Å /turn ideal helix



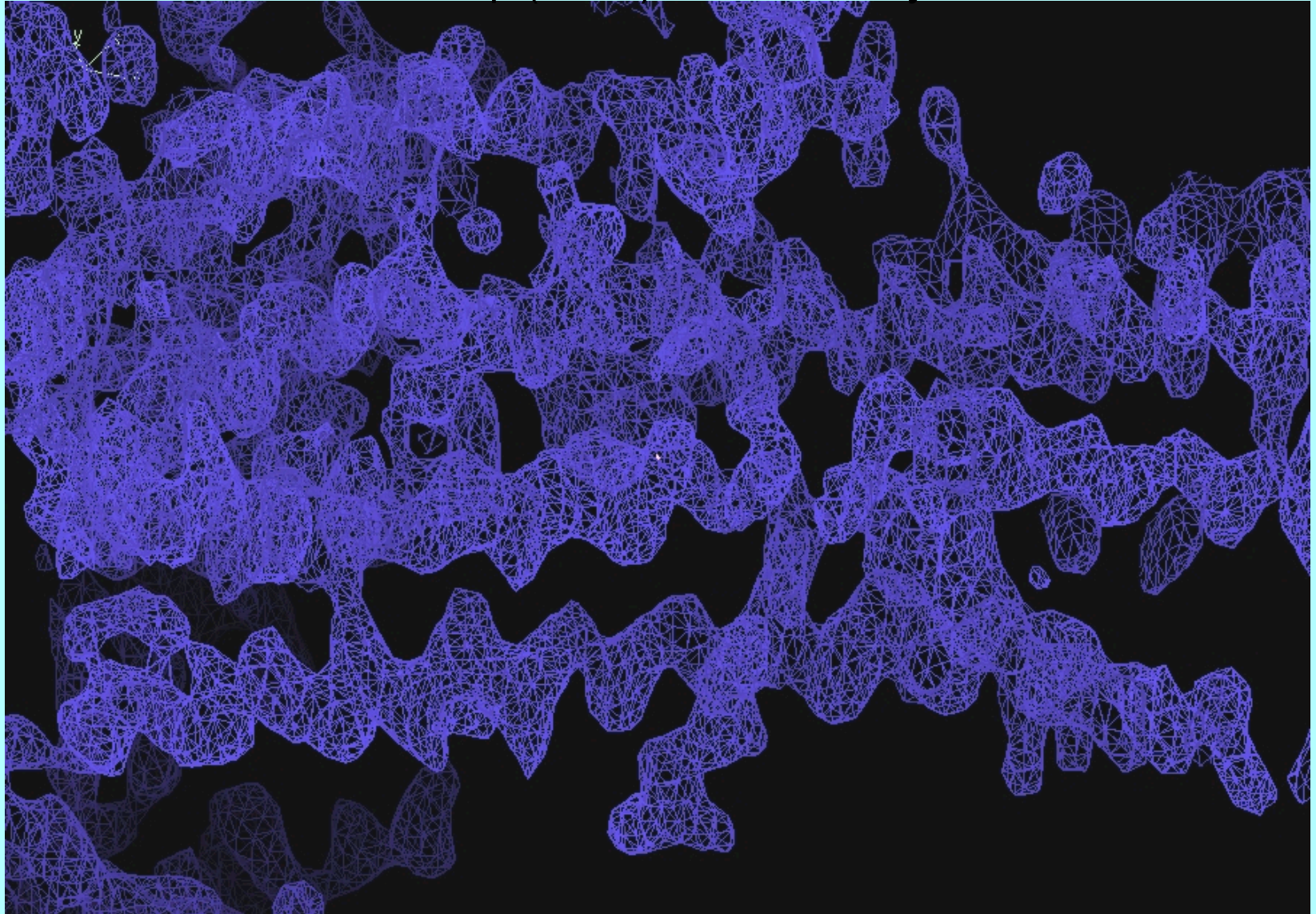
Identify direction and $C\alpha$ position from overlap with 4 Å radius helices offset ± 1 Å from main-chain

4 Å radius, 5.4 Å /turn ideal helix offset +1 Å along x

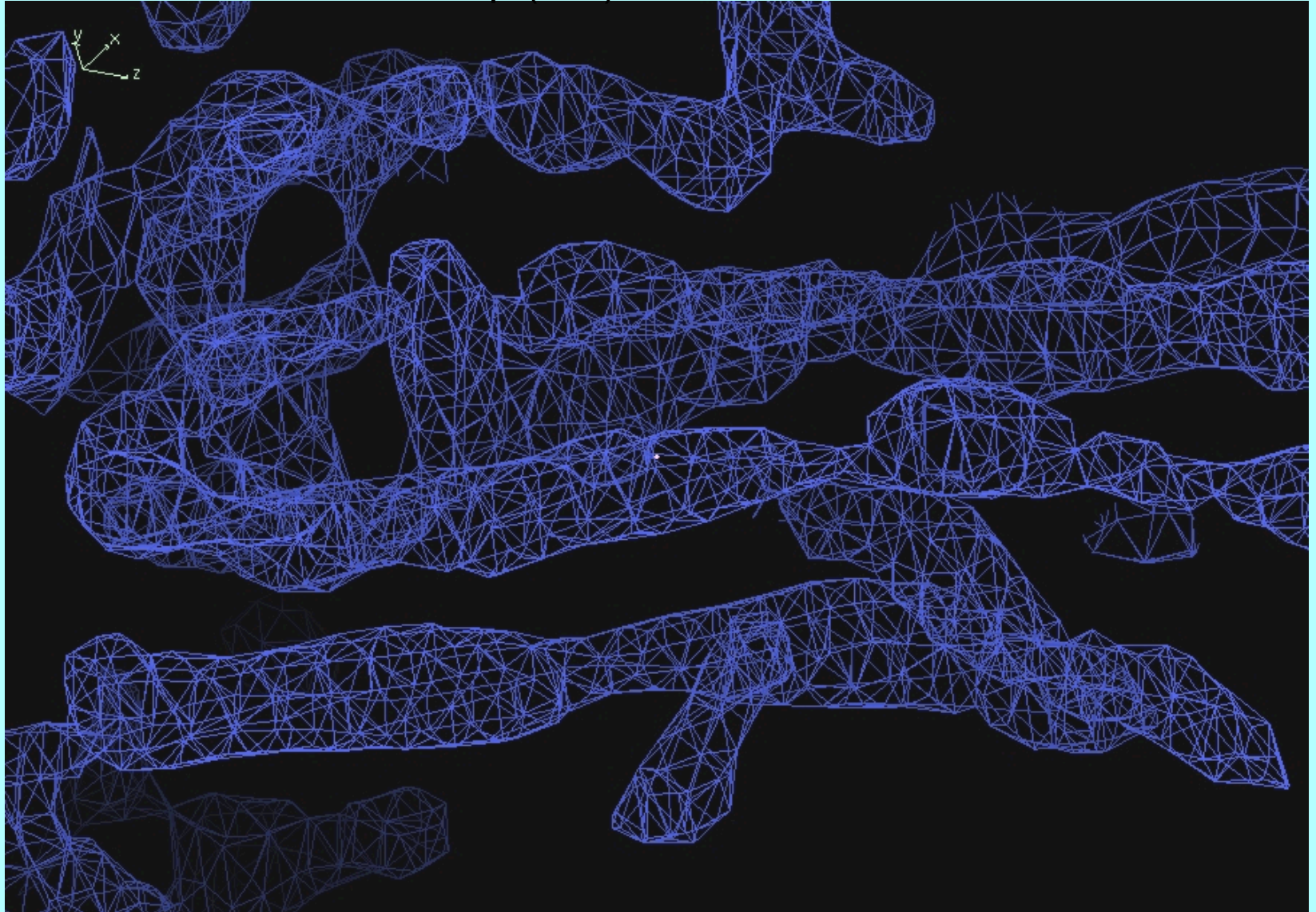


4 Å radius, 5.4 Å /turn ideal helix offset -1 Å along x

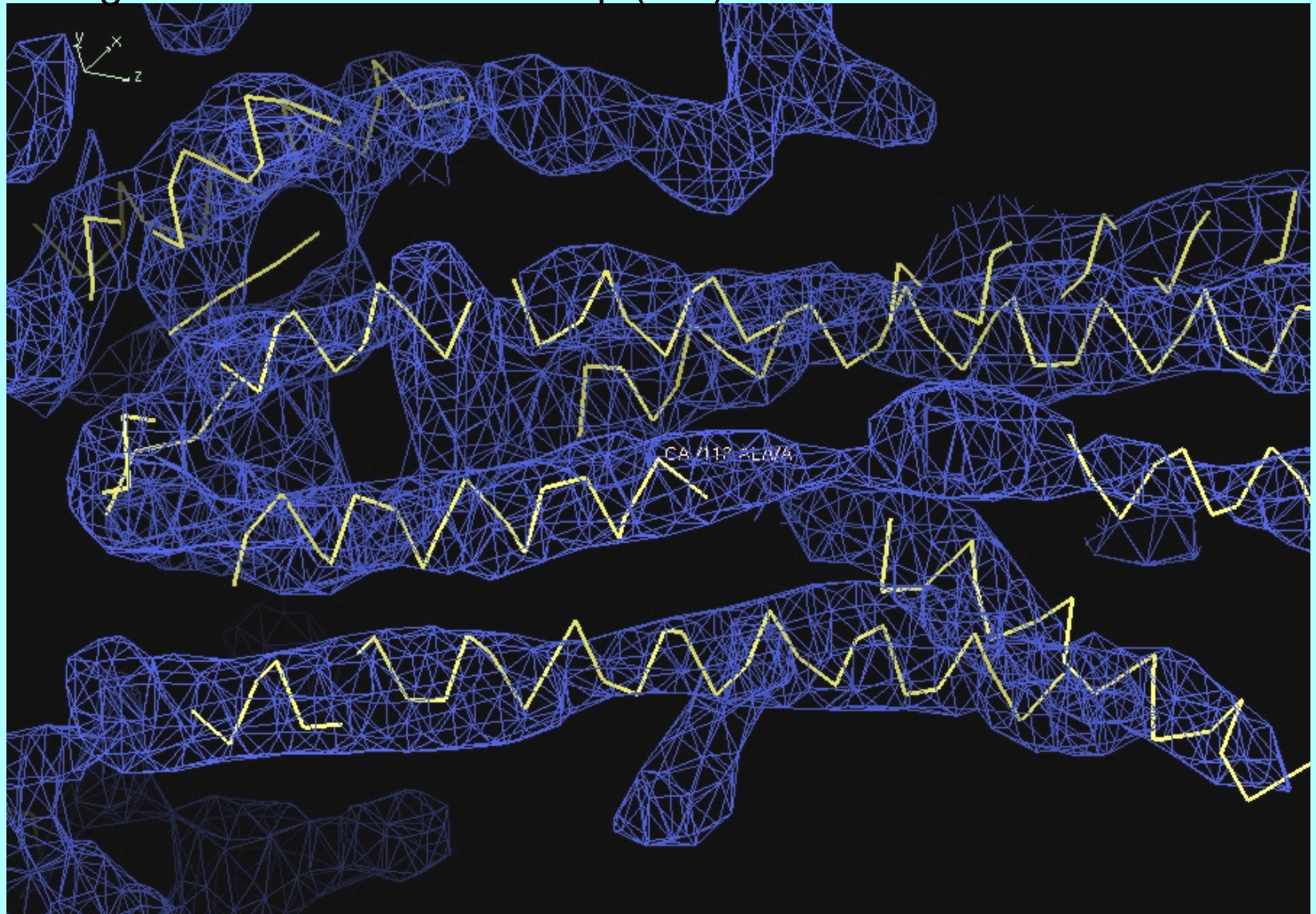
A real case: 1T5S SAD map (3.1 Å) Data courtesy of P. Nissen



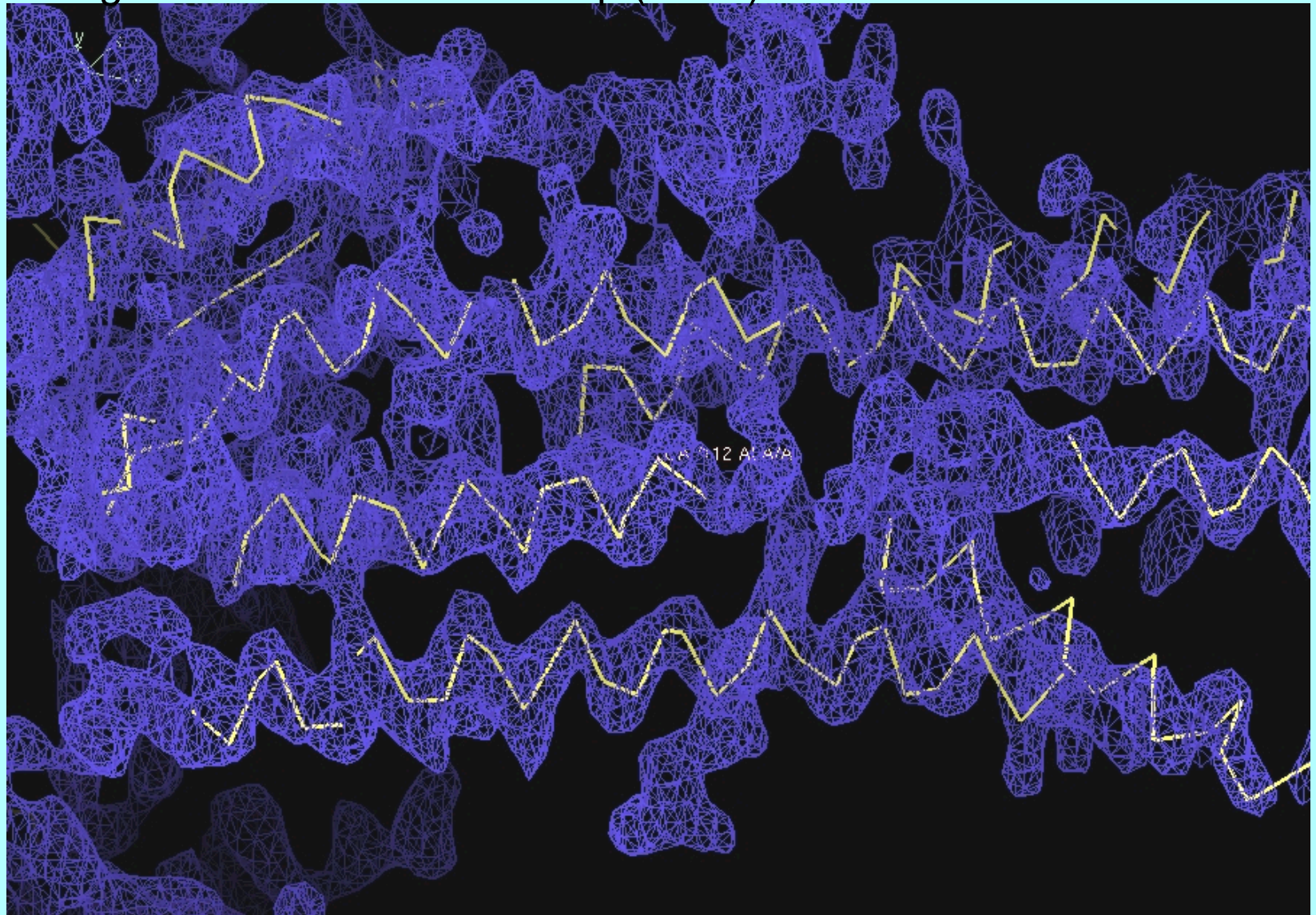
A real case: 1T5S SAD map (7 Å)



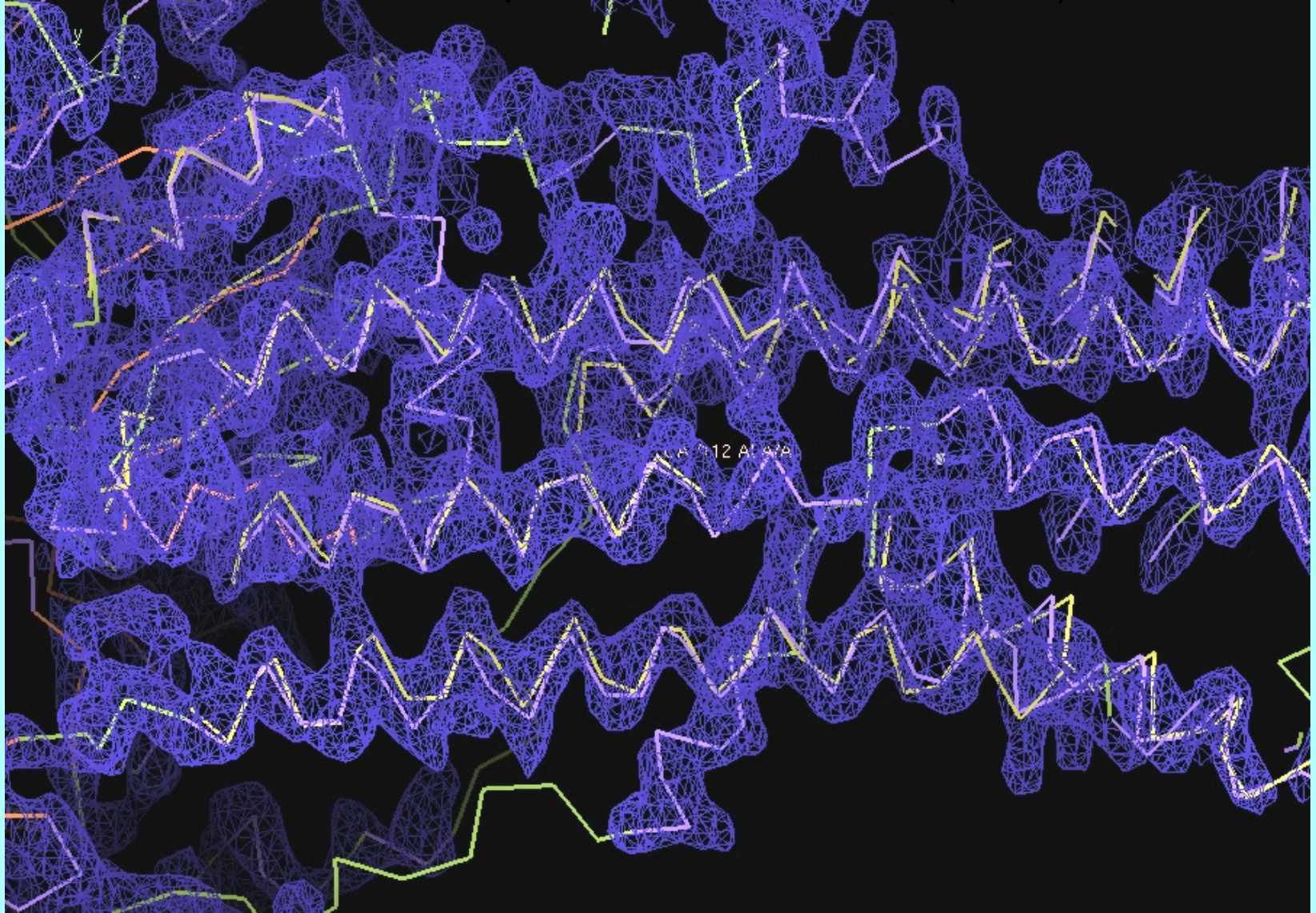
Finding helices in 1T5S SAD map (7 Å)



Finding helices in 1T5S SAD map (3.1 Å)



Helices from 1T5S SAD map compared with 1T5S (3.1 Å)



The PHENIX Project



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