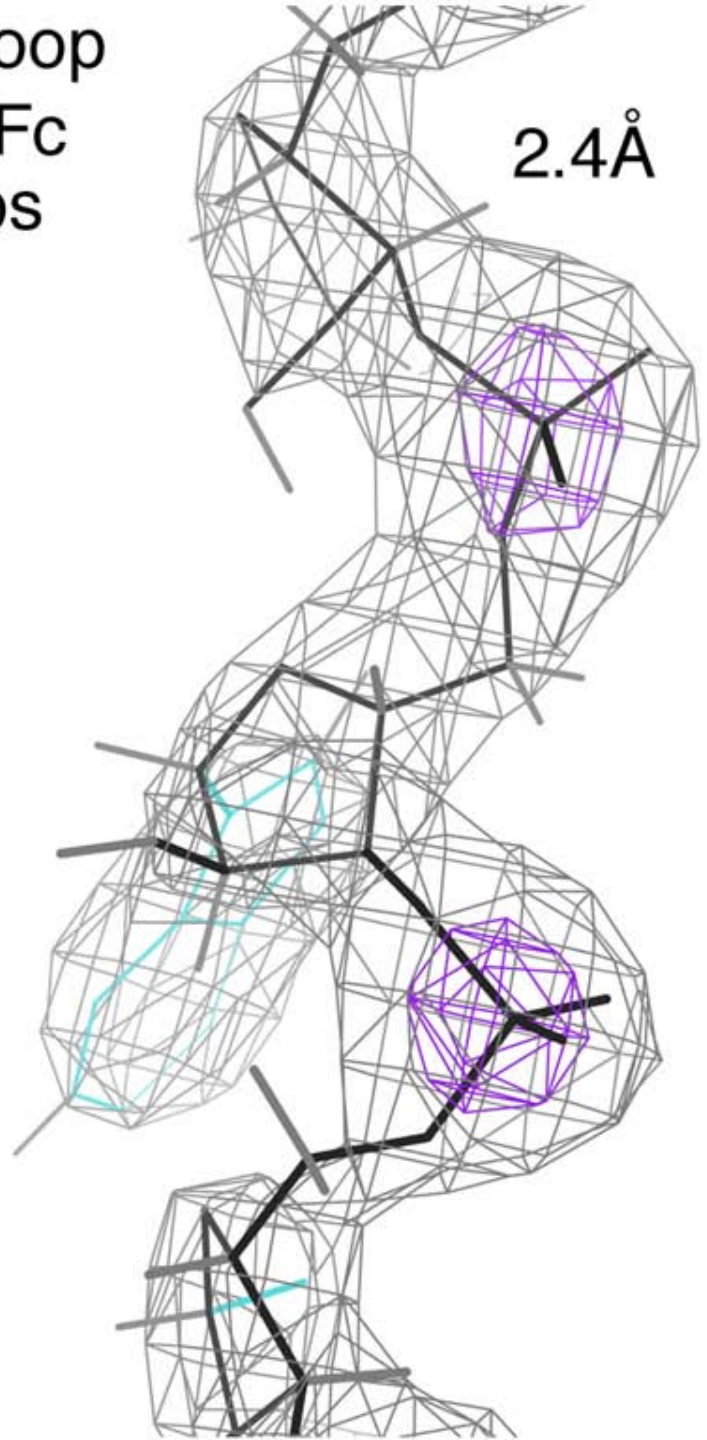
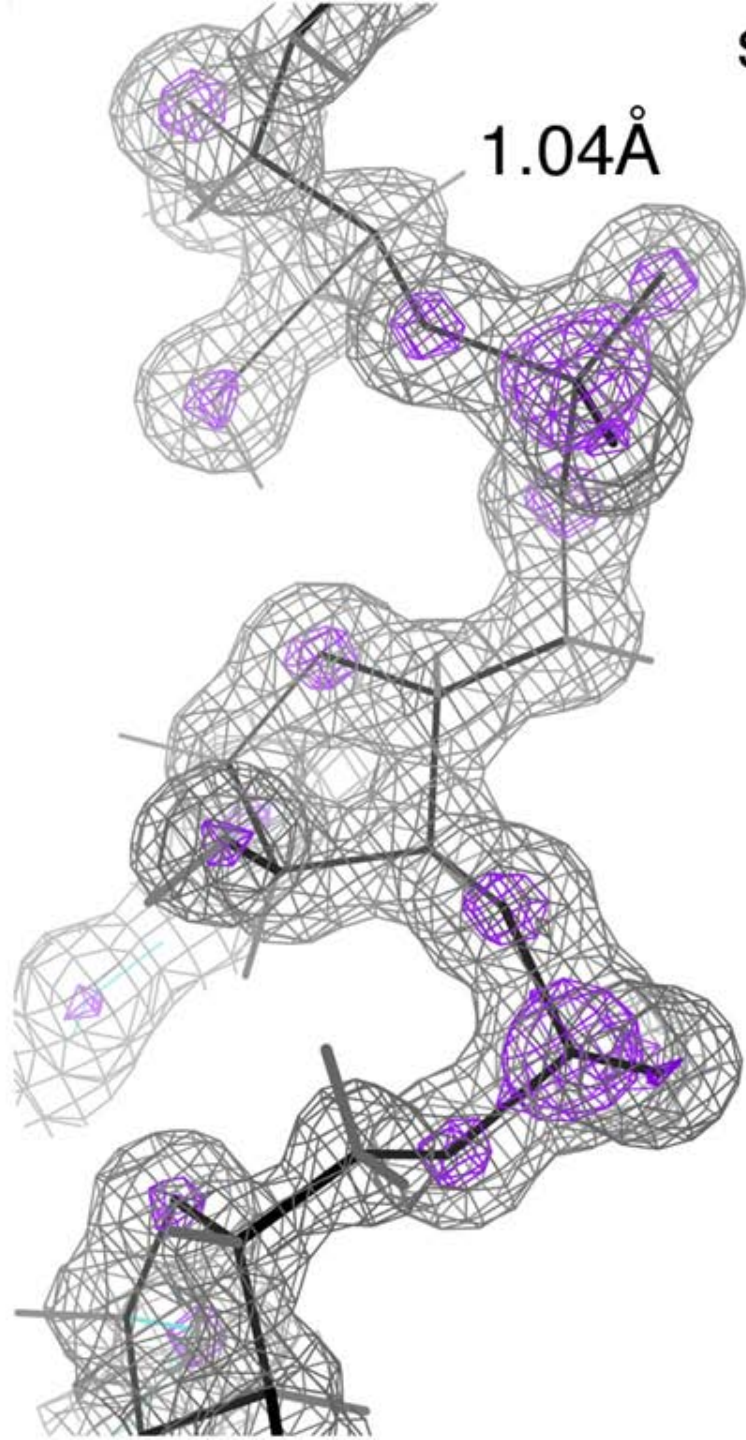
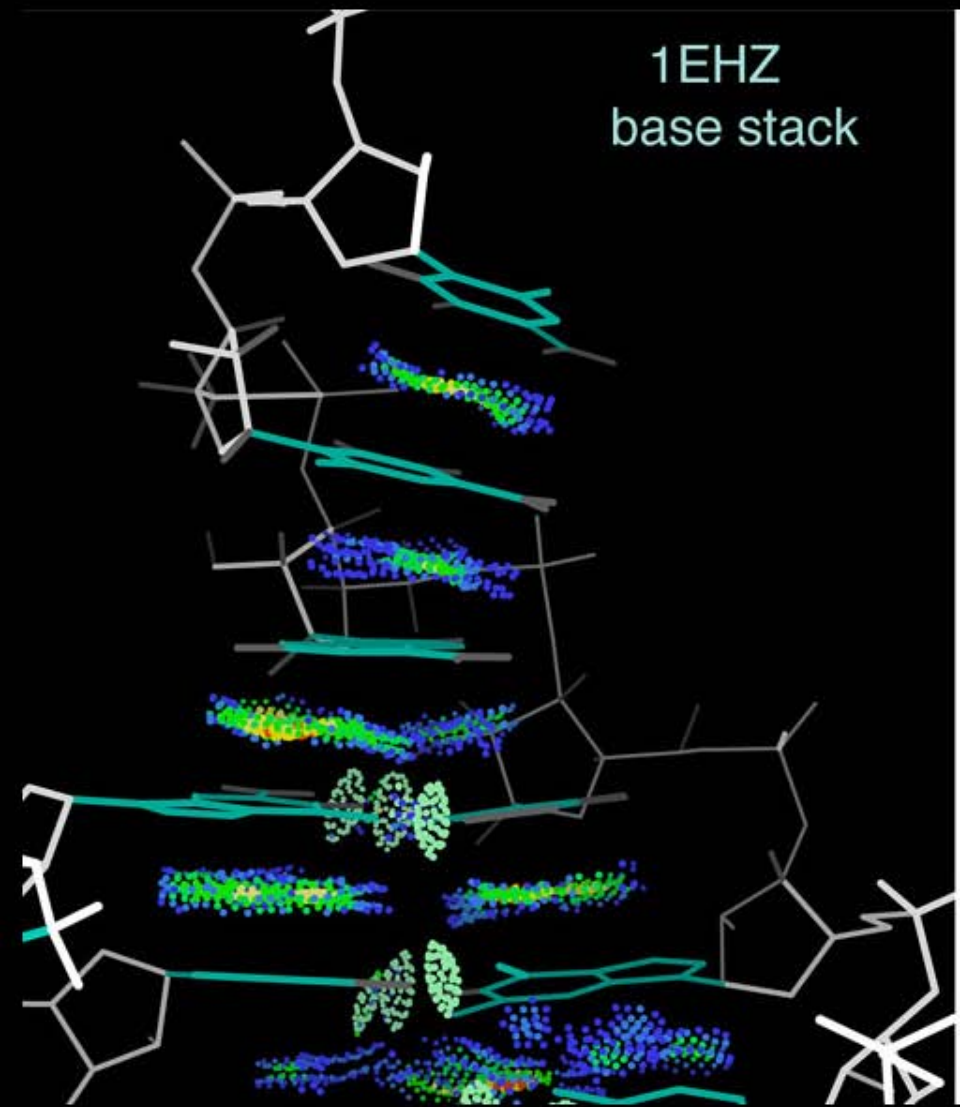


Too many variables!

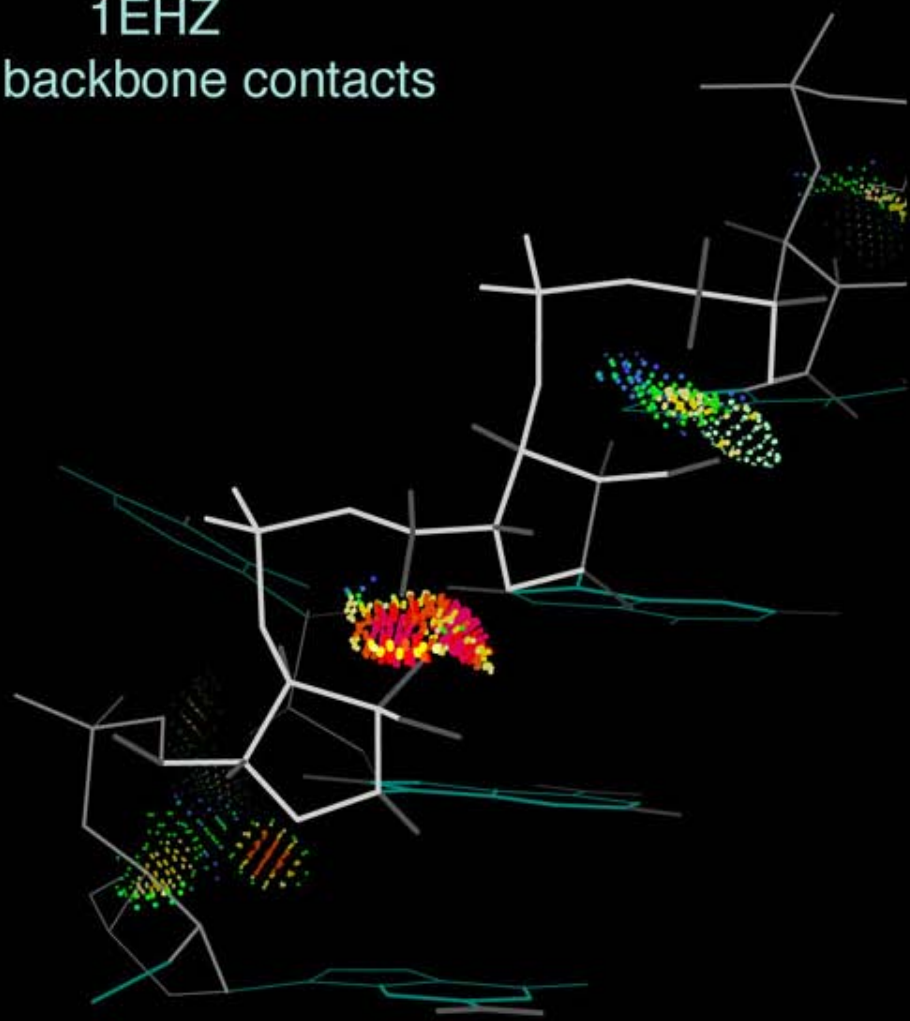
sarcin loop
2Fo-Fc
maps

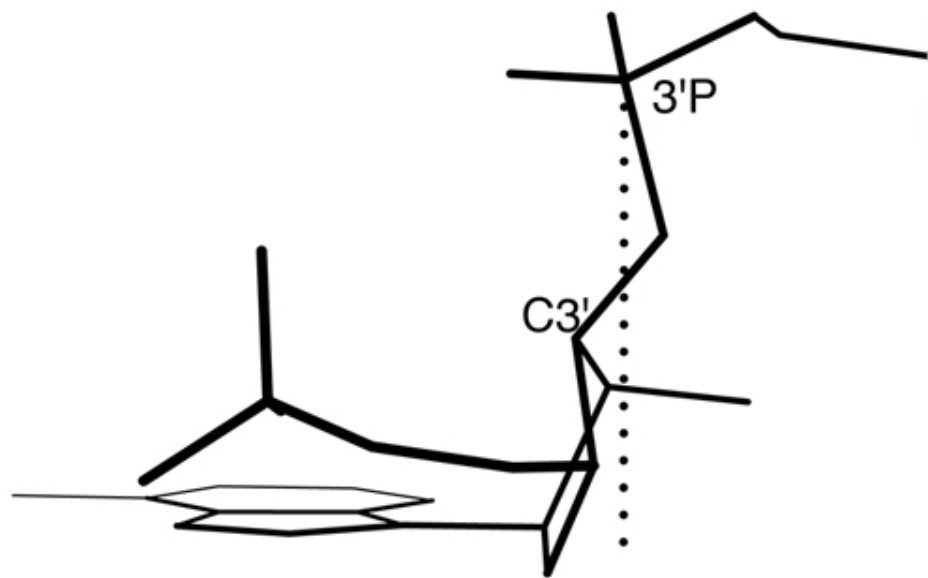


1EHZ
base stack

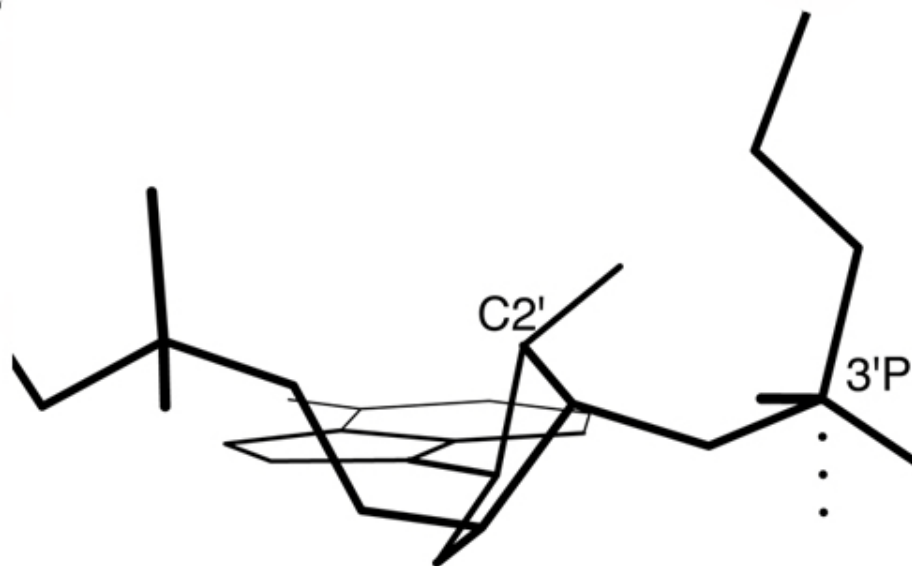


1EHZ
backbone contacts

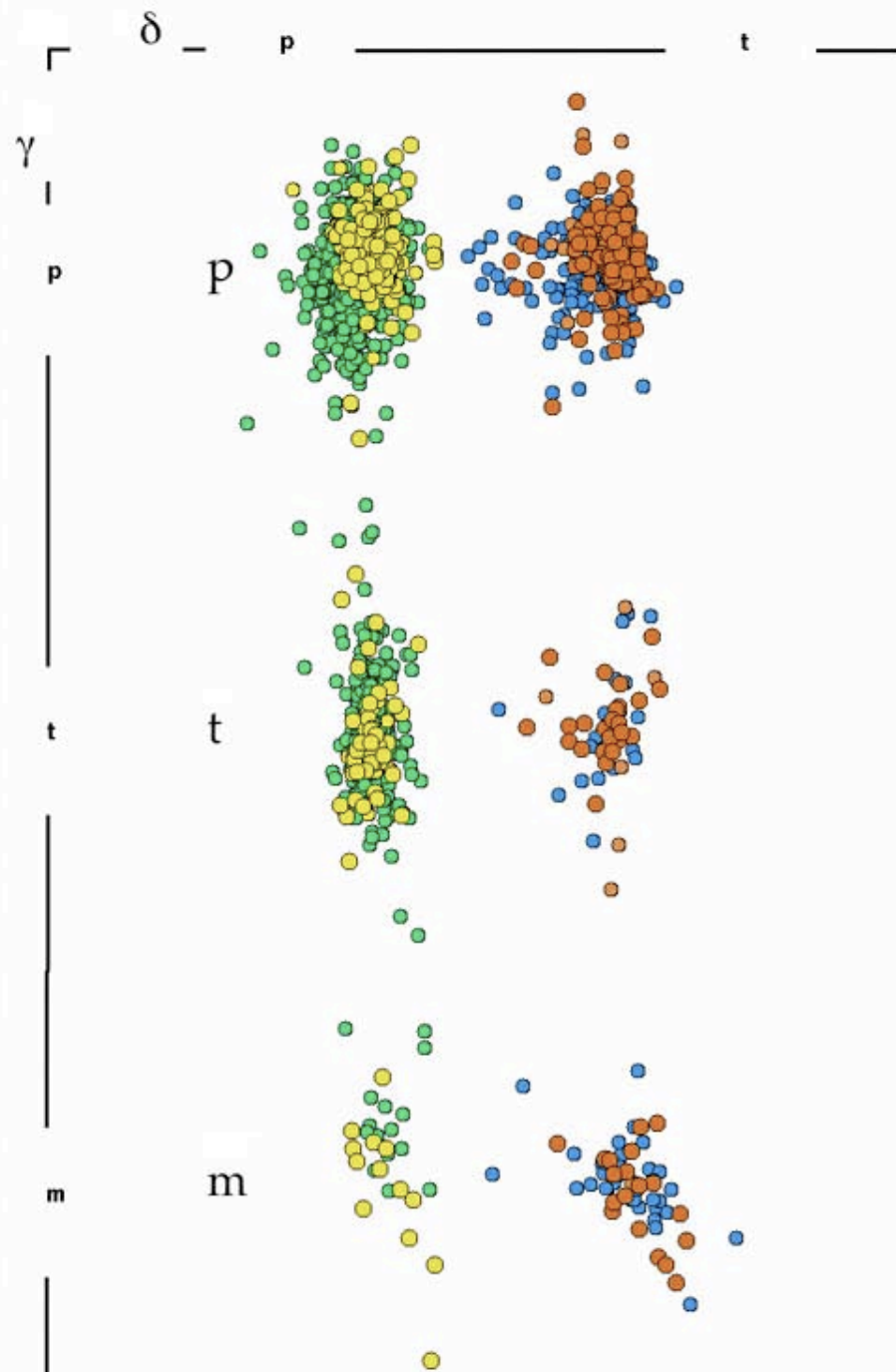
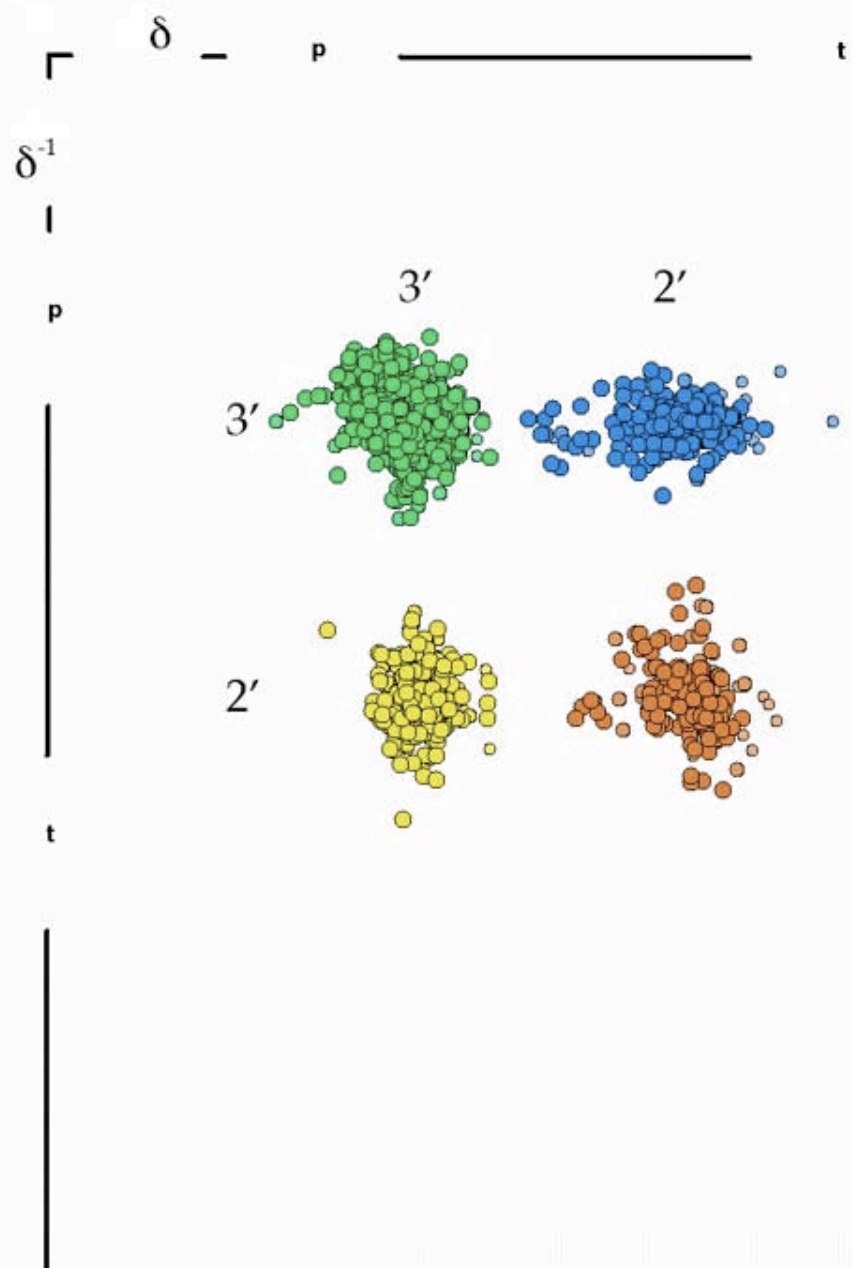


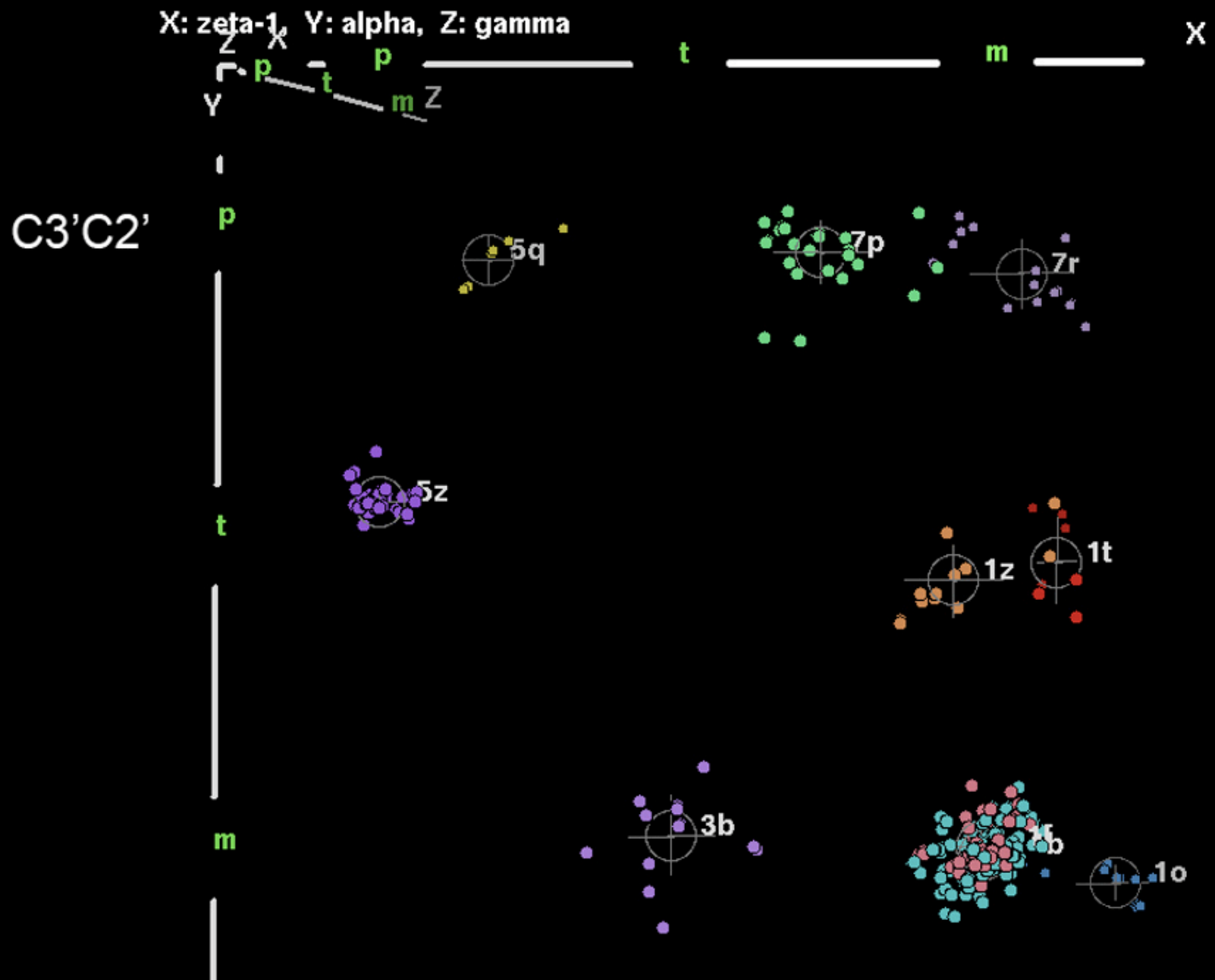


C3' pucker, long 3'P \perp



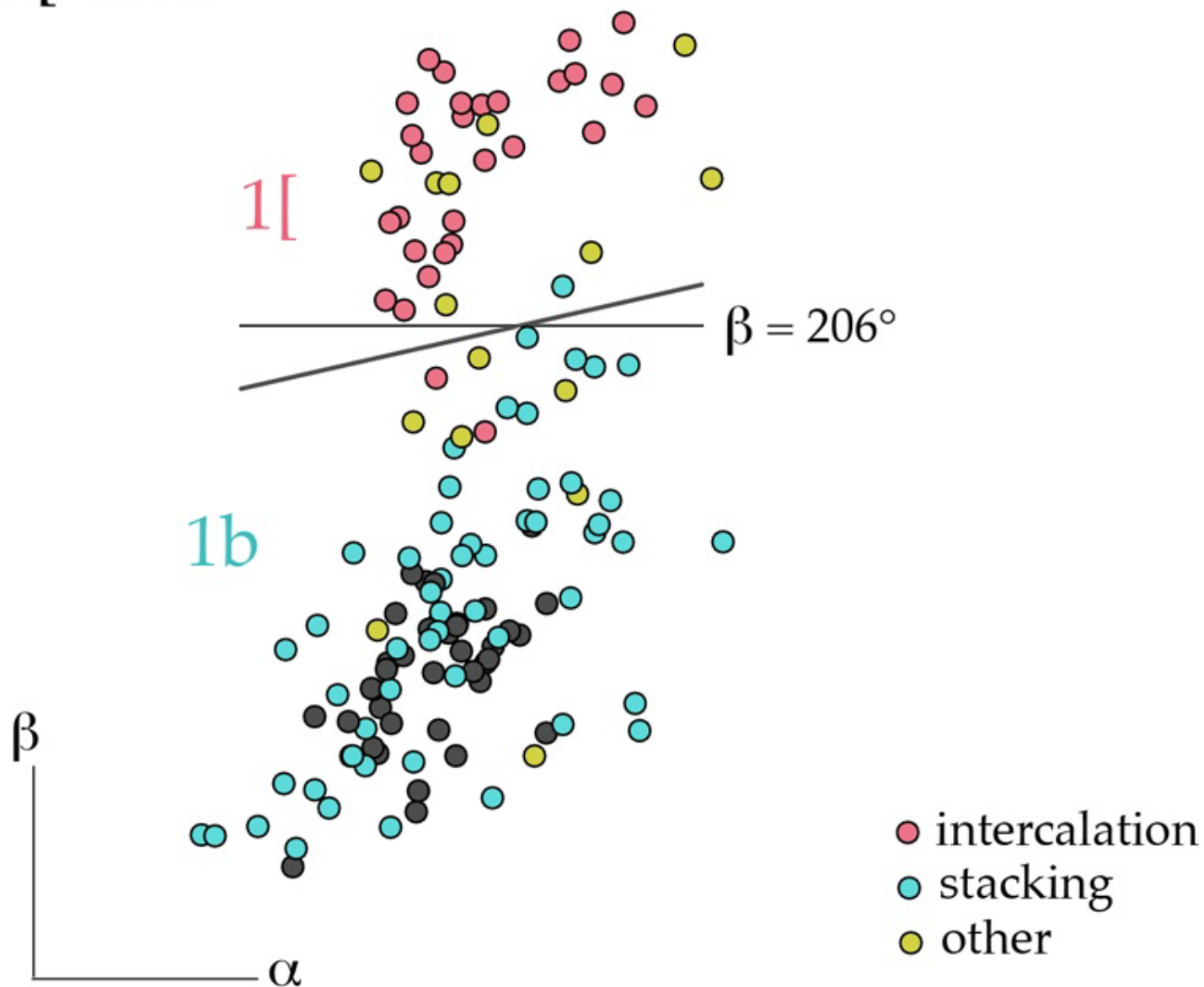
C2' pucker, short 3'P \perp

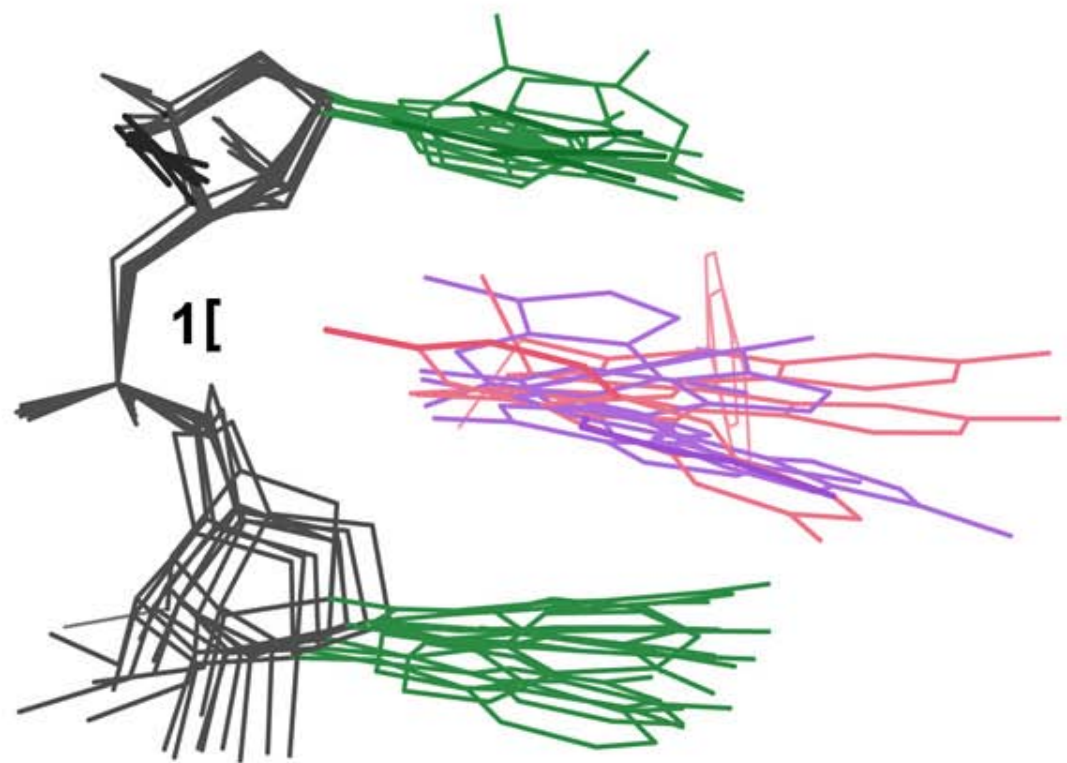
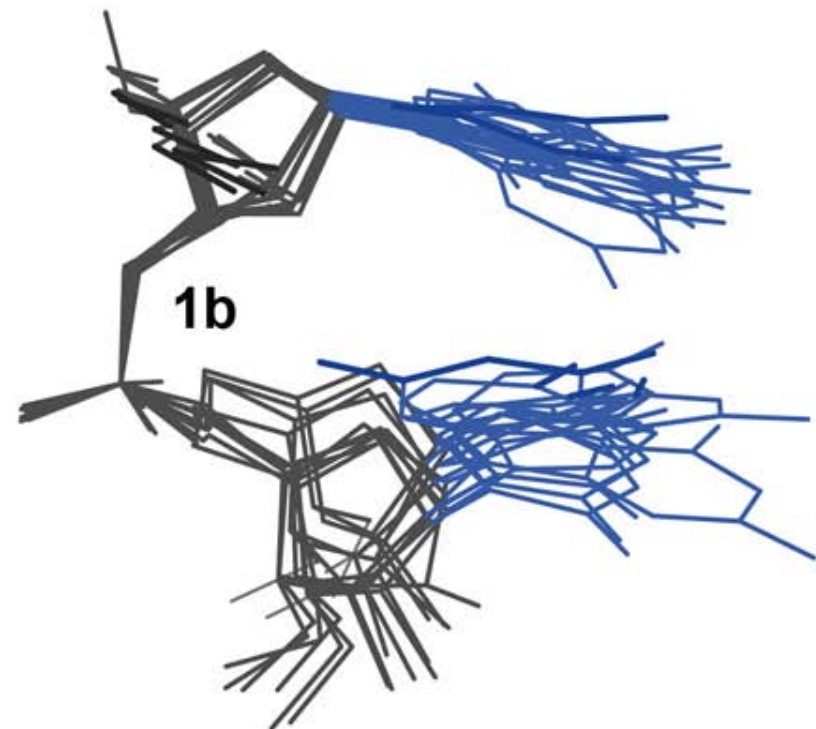


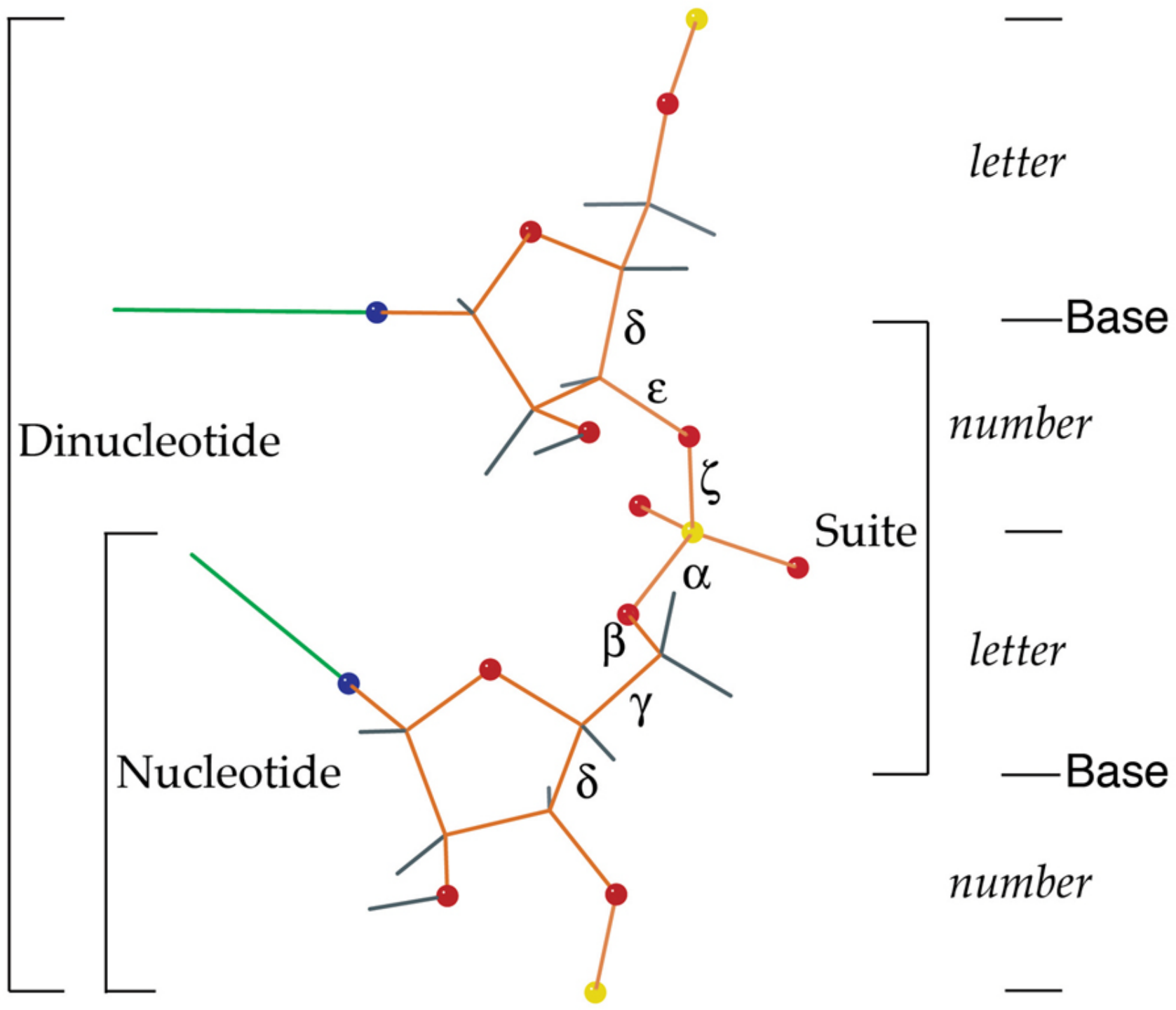


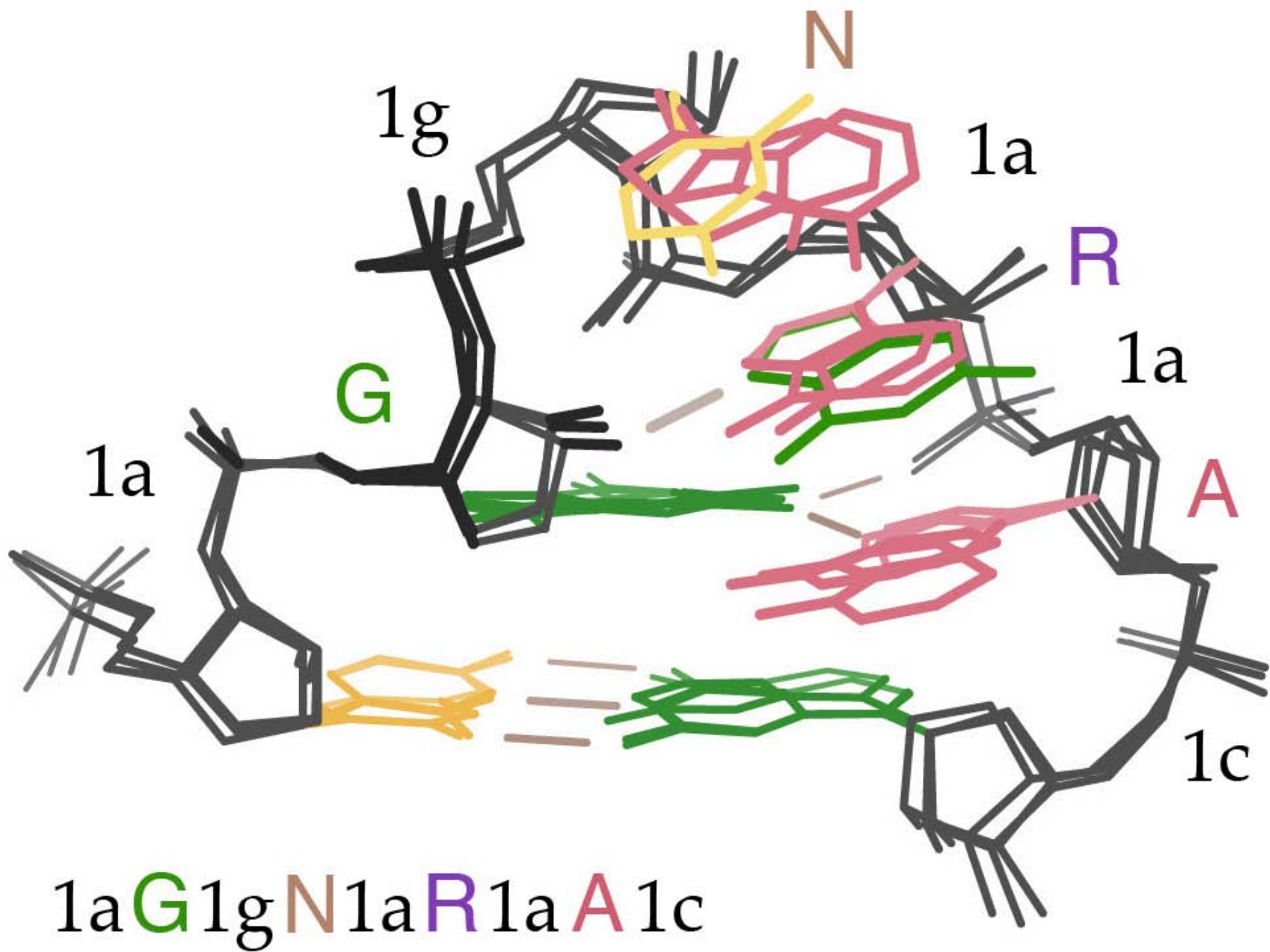
RNA backbone rotamer clusters, in 3 of 7D dihedral space

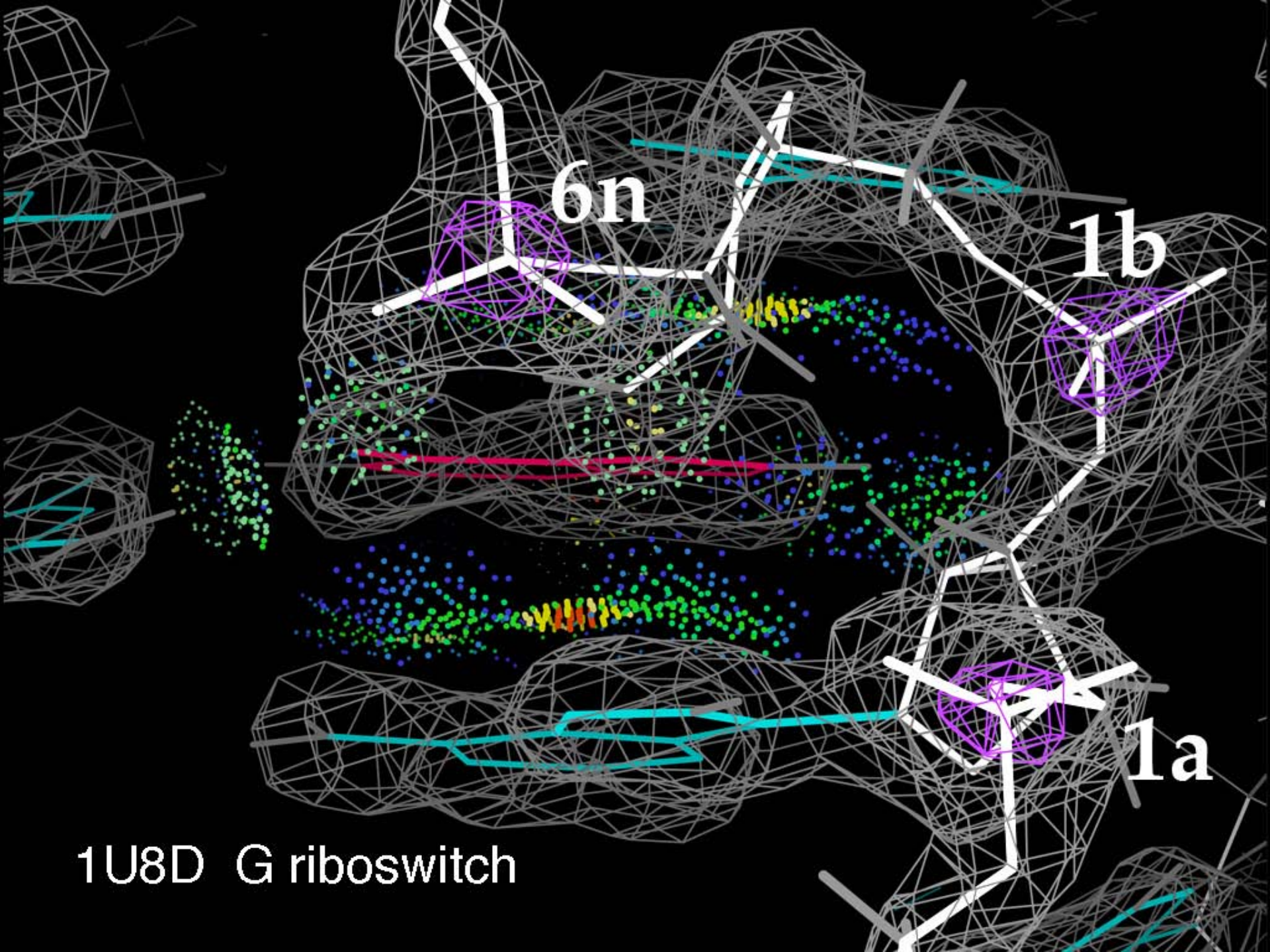
RNA Suite Conformations : clusters 1[& 1b











6n

1b

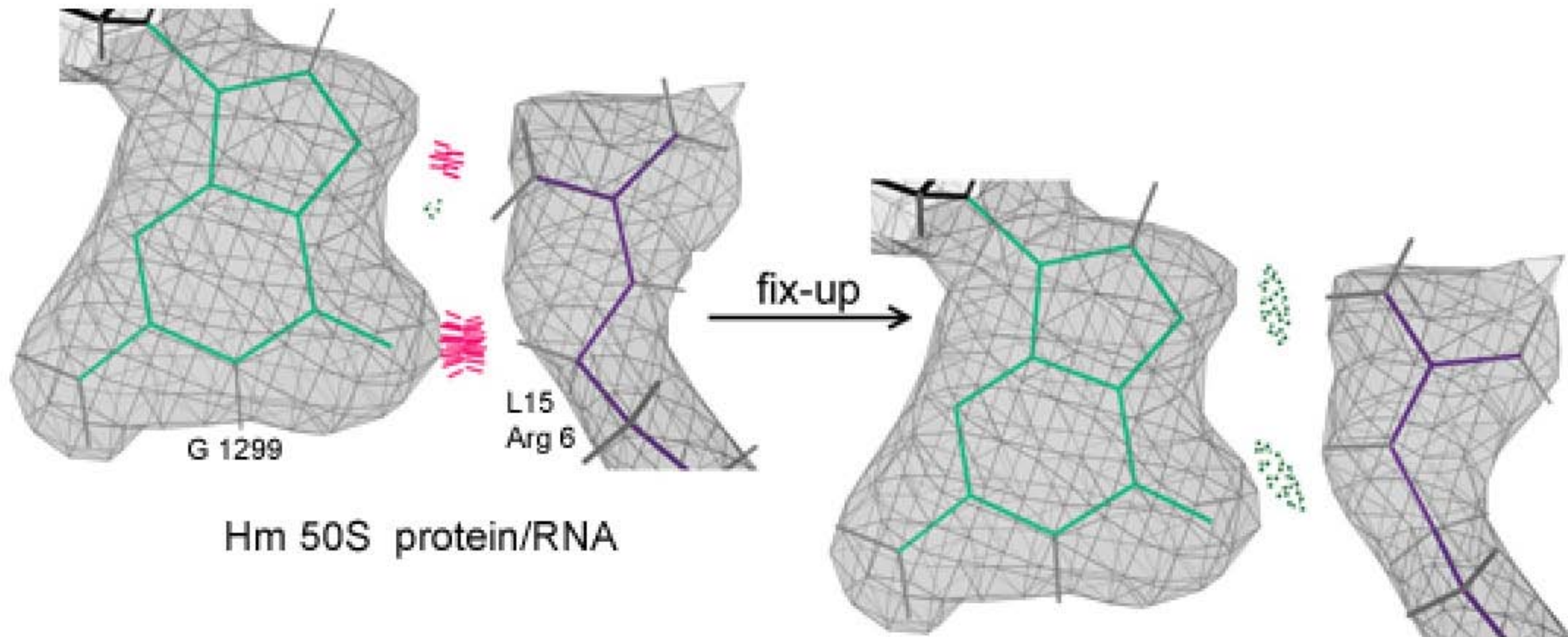
1a

1U8D G riboswitch

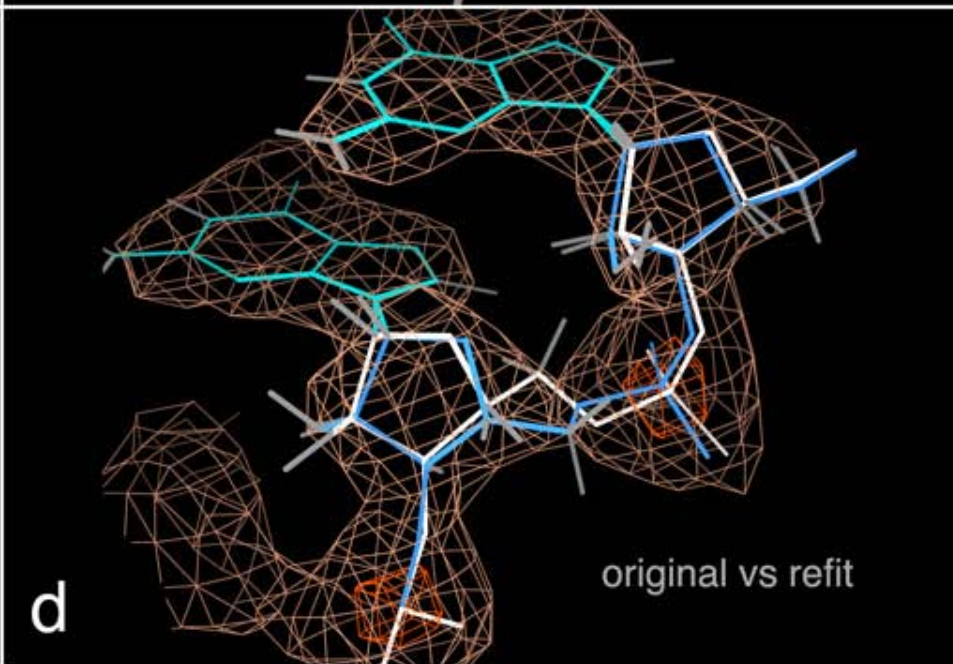
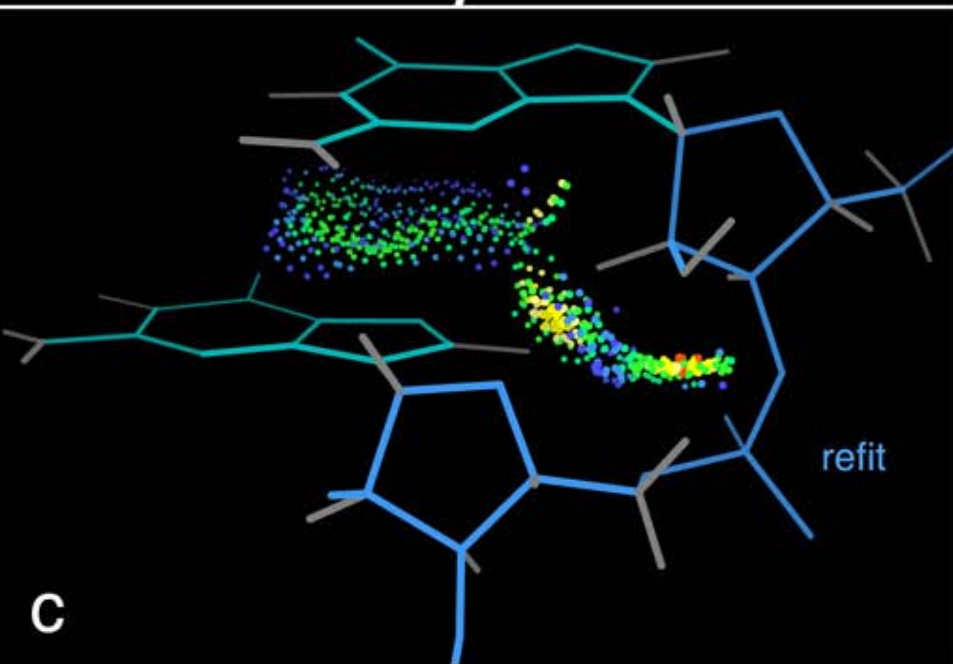
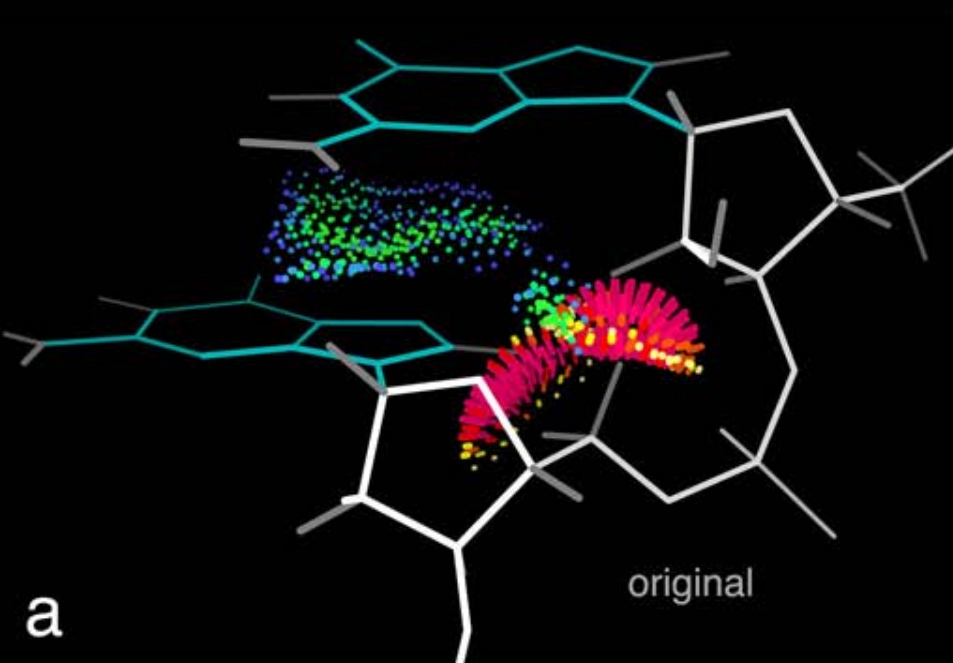
rr0082 / 1S72 rRNA partial suitestring, with **kink-turns** & **S-motifs**

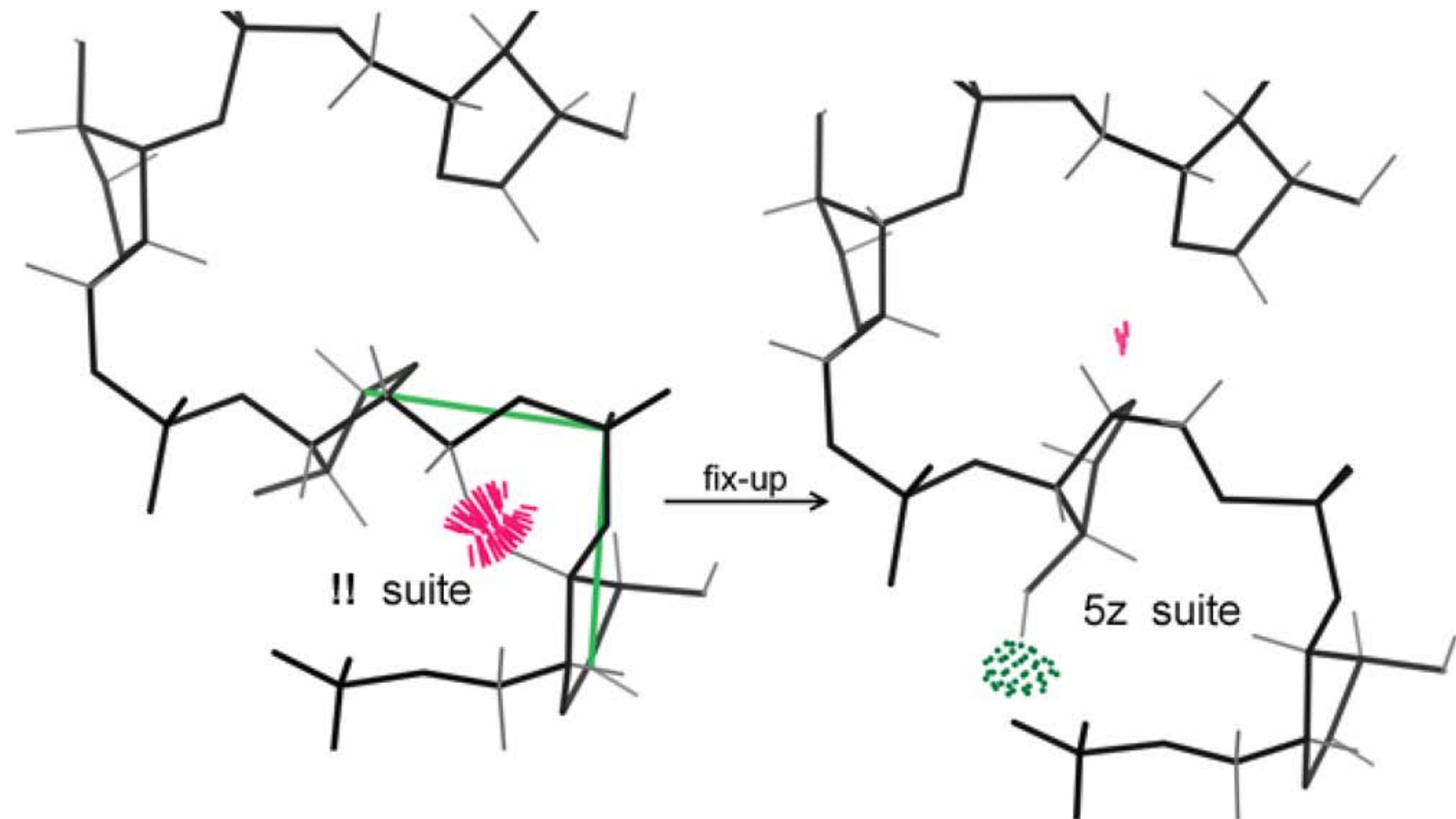
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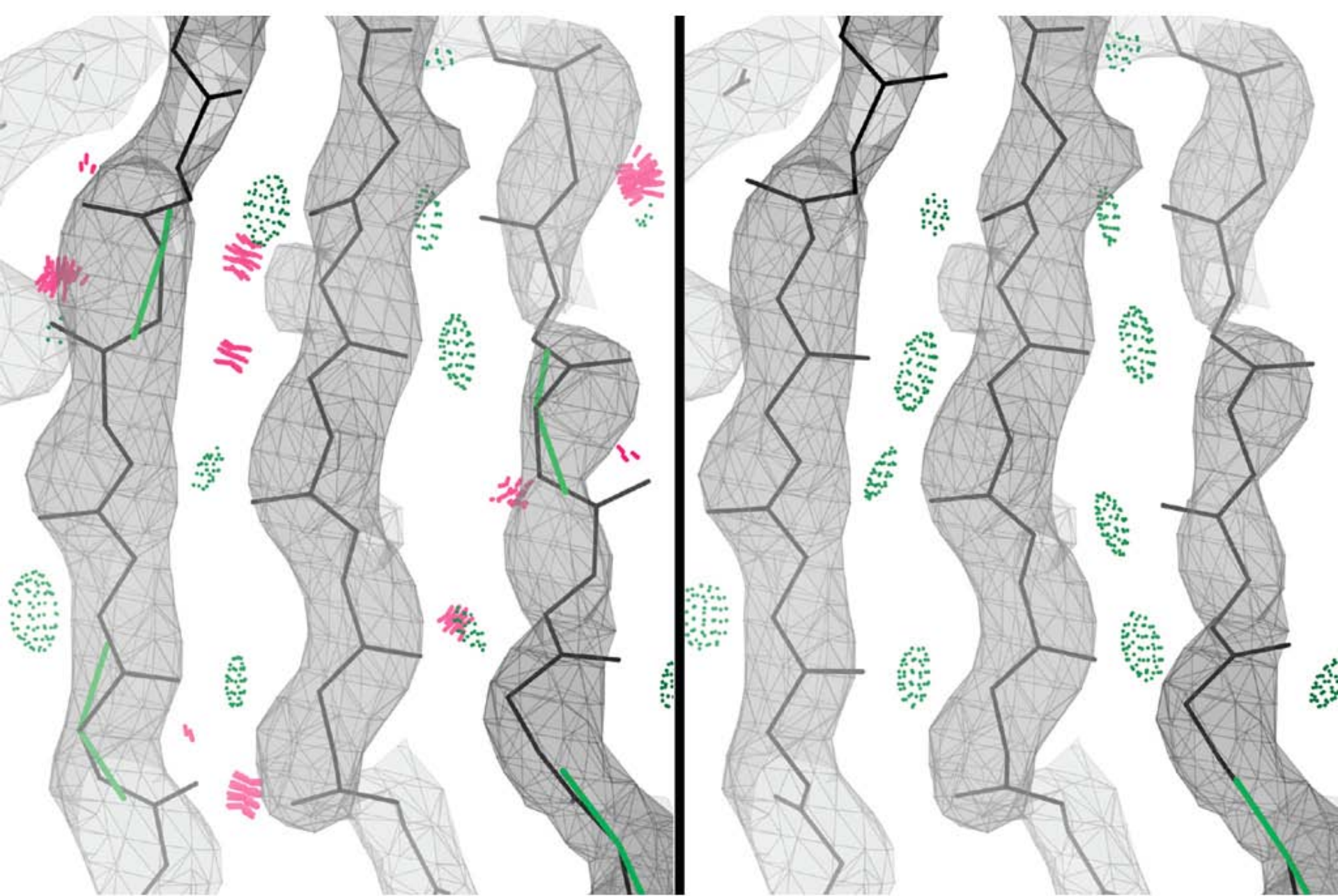


Arginines for RNA interfaces -- It is crucial to orient Arg guanidiniums right-side-up at RNA contacts

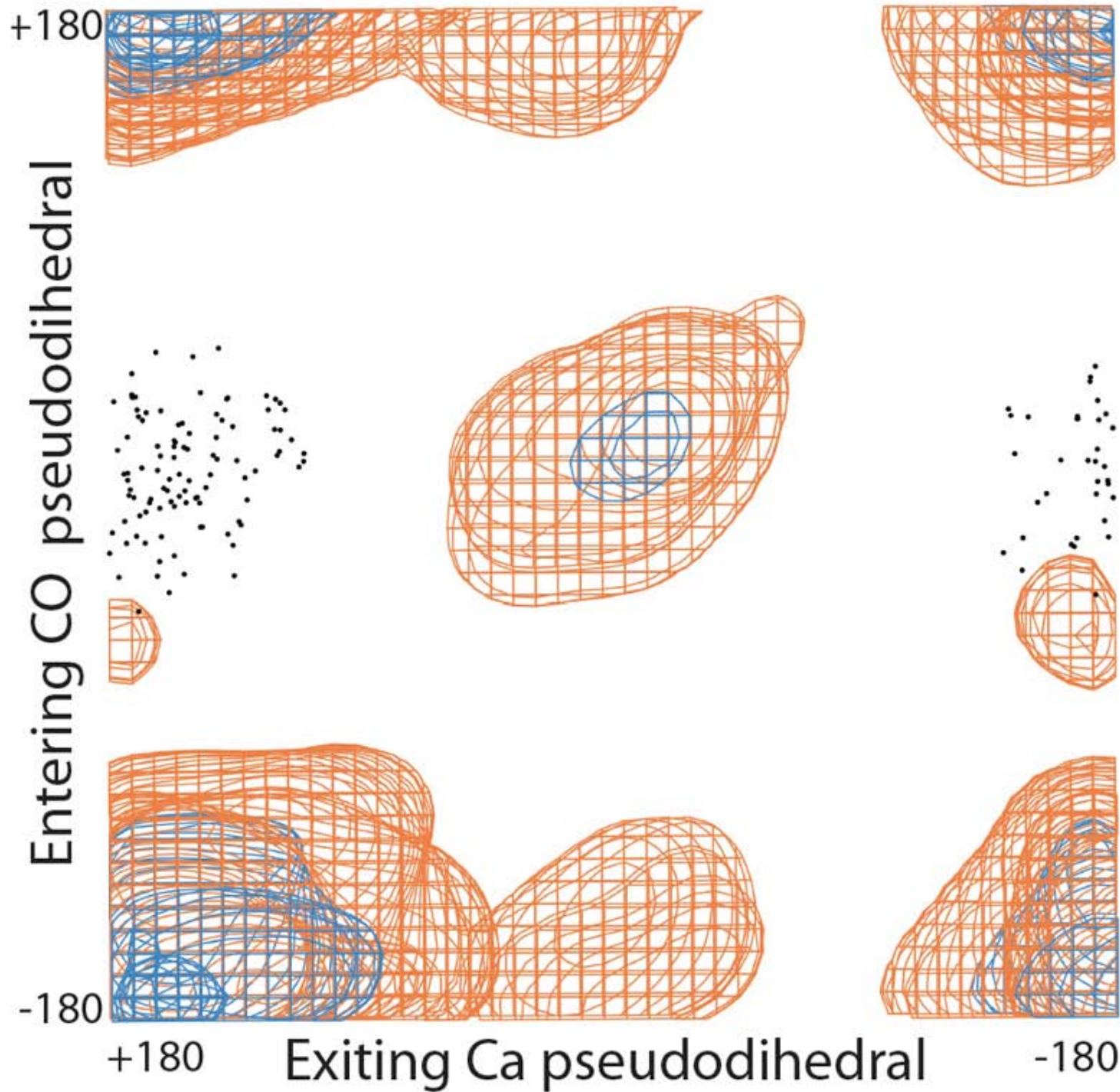


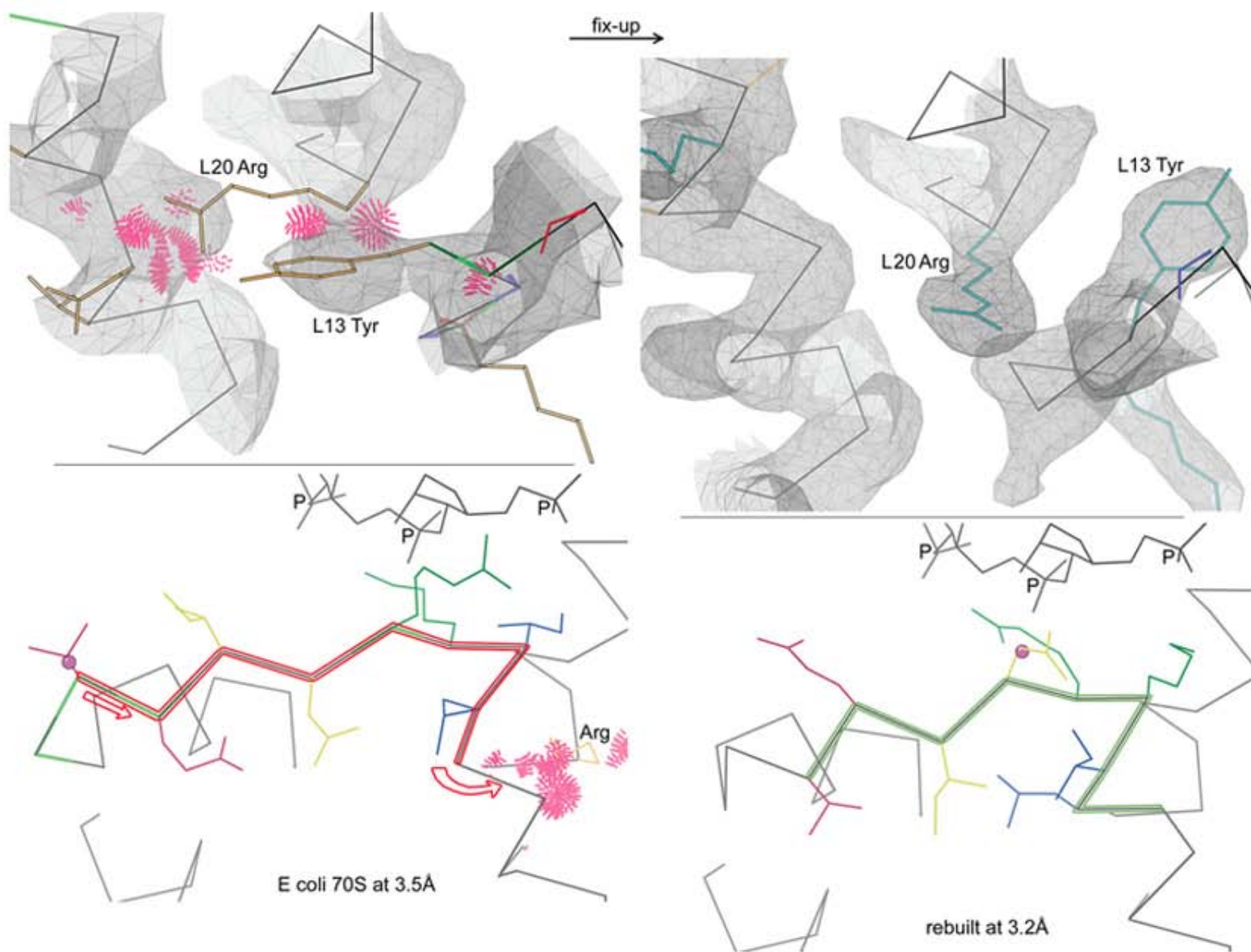


Fixing a non-helical RNA suite -- start of Smotif in Hm 5Srna



Ec70S: misfit β : **3 COs in same direction** -- vs corrected





Unraveling a case of error propagation -- In the initial 3.5Å maps, automated sidechain placement put Tyr 44 of protein L13 into good but incorrect density. Arg 63 of L20 was forced elsewhere, and found neighboring density where it distorted a turn of helix. This pushed nine residues of L20 over by one position, altering interactions with the RNA.

RNA Advances -

*Diagnosing puckers by 3'P perpendicular rule
Correcting ribose puckers & all-atom clashes
Evaluating backbone conformers
Pucker-specific parameters in PHENIX
Tighter geometry vs data weight*

Ribosome Refinements Difficult

*Even after good corrections, produce too
many bad bond & angle outliers*

(N.B. Also true of most RNAs in PDB)

*Now adding base-pair restraints & ties to
higher-resolution proteins*

We will persist - learning RNA & low-res





Protein crystallography

Structural informatics

MOLECULAR GRAPHICS

Protein de novo design

Packing: all-atom contacts

Validation & improvement

RNA BACKBONE

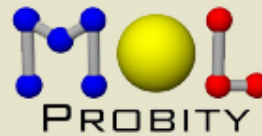
Folding, dynamics, NMR

Structure prediction: **CASP**

Building Tools & Concepts



All-Atom Contact Analysis



W. Bryan Arendall

Jeremy N. Block

Vincent B. Chen

Gary G. Kapral

Daniel Keedy

Christopher Williams

Swati Jain

Bradley Hintze

Lizabeth L. Videau

Michael G. Prisant

Jane & David Richardson

Ian W. Davis

J. Michael Word

Robert Immormino

Jeffrey J. Headd

Laura W. Murray

Jack Snoeyink
UNC

Bruce R. Donald
Duke

SECSG

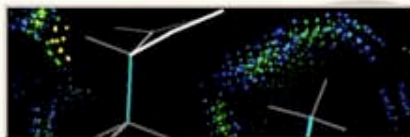
RNA Ontology Consortium

PHENIX project

NIGMS

3D Macromolecule Analysis & Kinemage Home Page at the Richardson Laboratory

Kinemages	RNA	Software	Databases	 MolProbity	Research	Teaching	Gallery	About Us
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Kinemages: 3D interactive graphics

"[The Mage Page](#)" discusses the what, where, and how of kinemage; some popular kinemage files are available from our [kinemage list](#), while more kinemages can be gotten browsing our [download section](#) ...

Software: Display & Contacts & Utilities

For those working with RNA: [RNABC](#) is updated and available for Mac OS X and [SuiteName](#) for RNA backbone conformer analysis is available either in MolProbity or as a standalone. Also, we added links to [collaborators' software](#) offerings; links are also available in the dropdown menubar.

Databases: protein & nucleic acid compilations

Top500 angle dataset ([top500-angles.050606.zip 80MB](#)) & [README](#) for Ramachandran contours and rotamer scoring distributions, [Top500](#) proteins with optimized H atoms, [rotamer libraries](#), [RNA backbone rotamers](#), ...

MolProbity: structure validation

Web service for all-atom contact and geometrical analysis of your model. Click this section's header, the image at left, or the MolProbity badge in any of the menus to go to the initial page of the MolProbity server.

Research: 3D structure of proteins & nucleic acids

[All-atom contacts](#); structure validation & improvement; protein backbone motions; protein sidechain rotamers; [RNA backbone rotamers](#), or view the RLab research index page.

Teaching: Course materials

Duke courses: [BCH222](#), [BCH258](#), [BCH291](#), & [CHEM22L](#).
Off-site workshops: [on-line tutorial](#) on validation and rebuilding (updated from the 2005 ACA convention short course); [CSH X-Ray Course](#), annual course; and [others](#).

Gallery: images

Take in our [2D images](#) and 3D kinemages. View the on-line [HTML version](#) of the annotated Anatomy and Taxonomy of Protein Structure, or download the PDF pages.

About us: Lab Info

(very) Odds n' (no) Odds re. RLab: [lab members](#), [directions to the lab](#), [select publications](#), [lab wiki](#), lab links & partners in quality: [PHENIX](#), [ROC \(RNA Ontology\)](#), [SECSG](#), [Duke Biochem. Dept.](#), [Duke SBB program](#)