



Riboswitch 3D prediction

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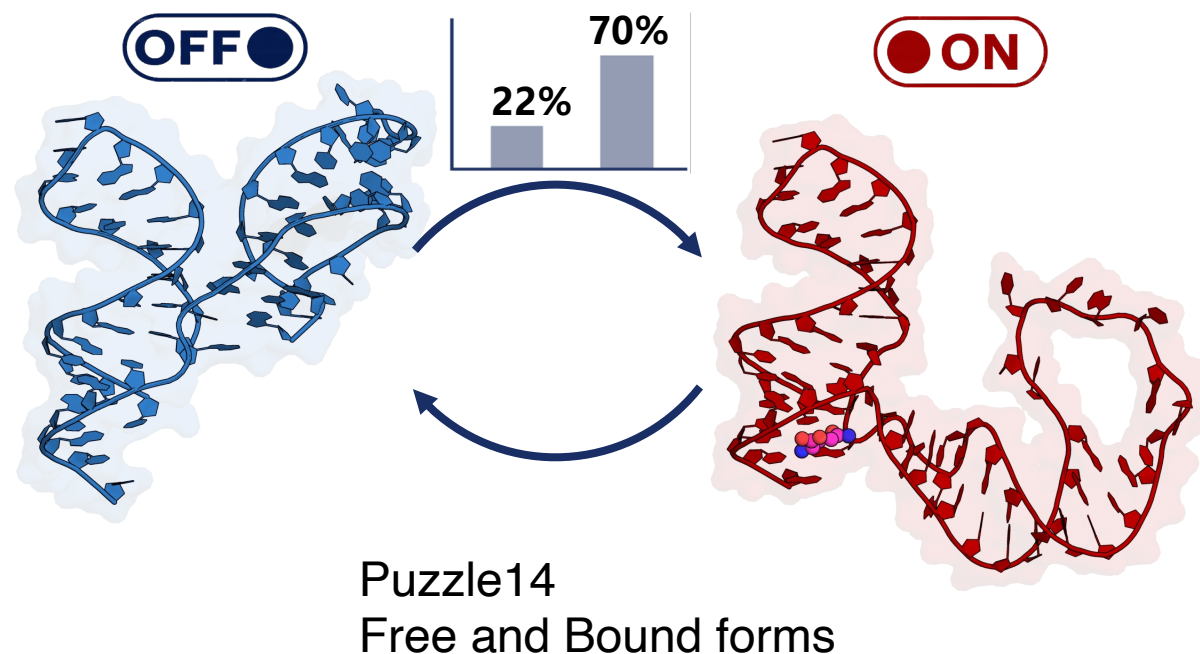
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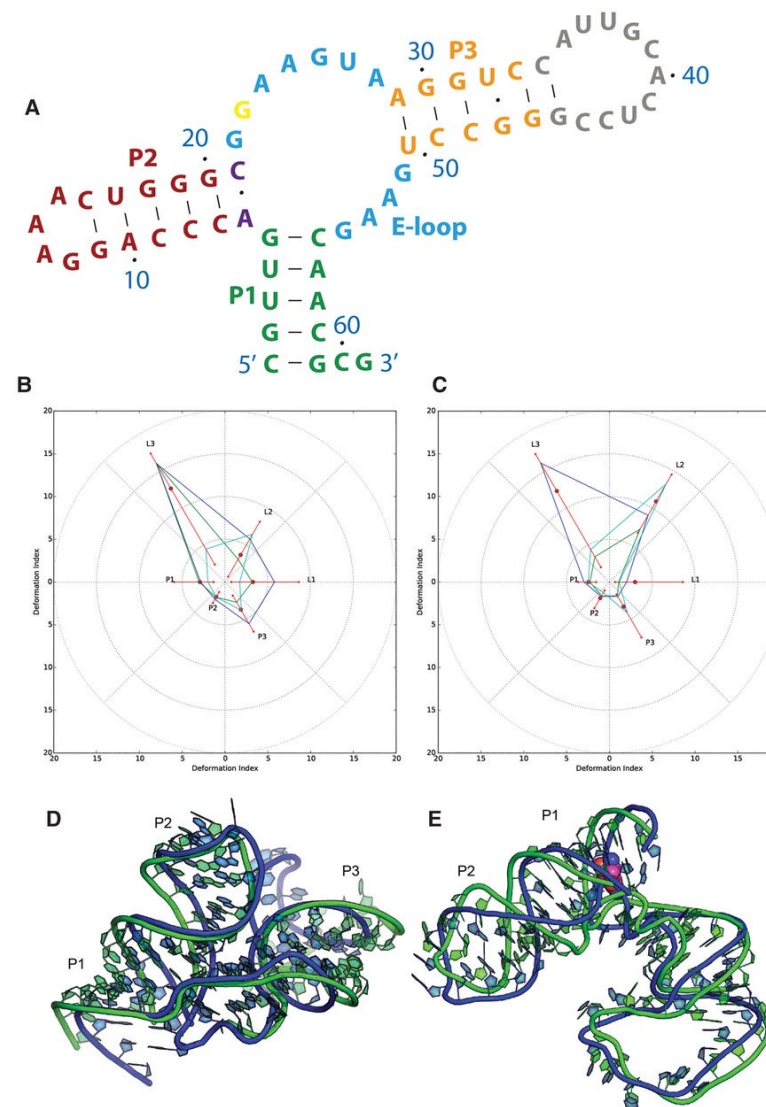
Riboswitches are conditional folds. Predict the condition, then the coordinates.



Why RNA 3D prediction matters



Binding pocket + regulatory platform



Ribocentre-switch: a riboswitch database



GZNL's Respiratory Data Centre, GZNL-RDC

Ribocentre-switch

A database of riboswitches

Example: Mg Orphan SAH Riboswitches Sequences THF Teams

Home Riboswitches ▾ Download ▾ Binding pockets Applications Publications Help

Azaaromatic

- Guanidine-I
- Guanidine-II
- Guanidine-III
- Guanidine-IV

Amino acids

- Glycine
- Lysine
- Glutamine-I
- Glutamine-II

Elemental ions

- Fluoride
- Mg²⁺-I
- Mg²⁺-II
- Mn²⁺
- NiCo
- Na⁺-I
- Na⁺-II
- Li⁺-I
- Li⁺-II

Others

Sugars

- GlcN6P

Cofactors

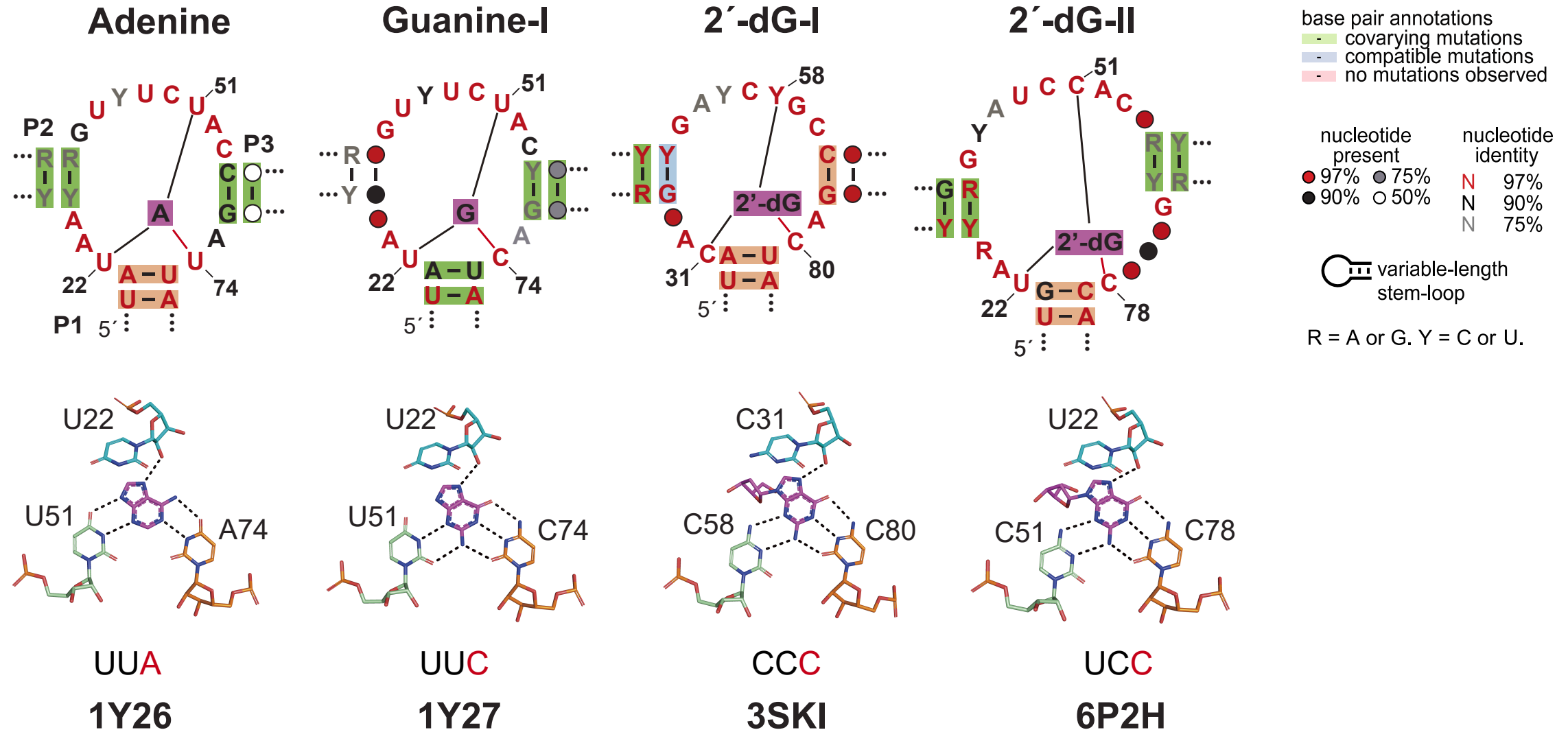
- AdoCbl
- MoCo
- THF-II
- SAM-I
- SAM-II
- SAM-VI
- NAD⁺-I
- AqCbl
- Wco
- TPP
- SAM-IV
- SAM-V
- SAM-SAH
- NAD⁺-II
- FMN
- THF-I
- HMP-PP
- SAM-I/IV
- SAM-III
- SAH

RNA derivatives

- Xanthine-I
- Xanthine-II
- 2'-dG-I
- 2'-dG-II
- 2'-dG-III
- PreQ₁-I
- PreQ₁-II
- preQ₁-III

<https://riboswitch.ribocentre.org/>

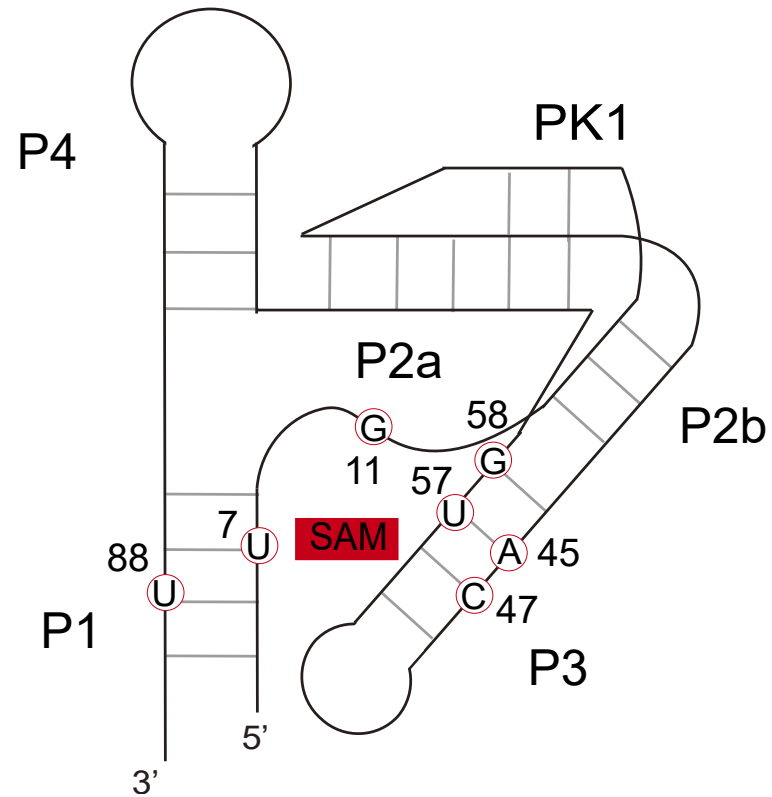
Common binding mechanism in the binding pocket



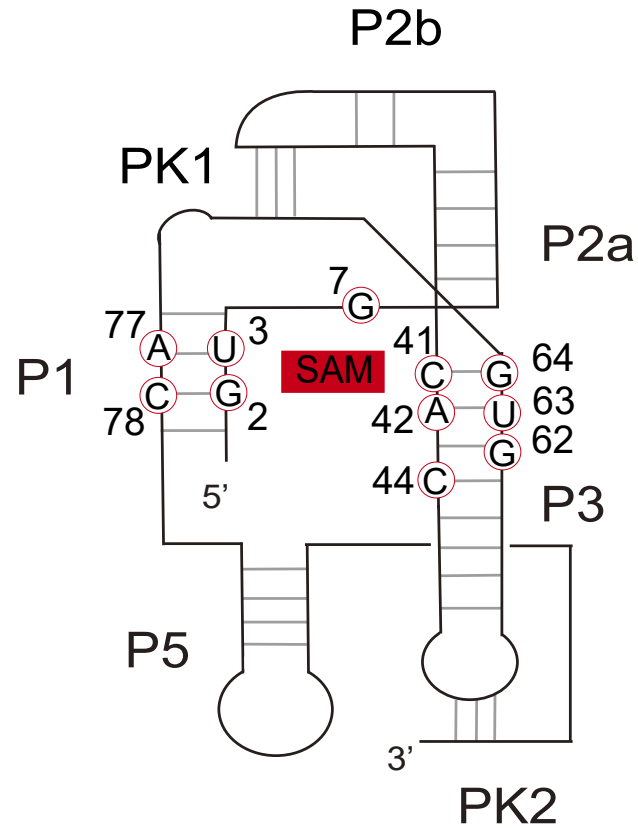
Conservation in the binding pocket



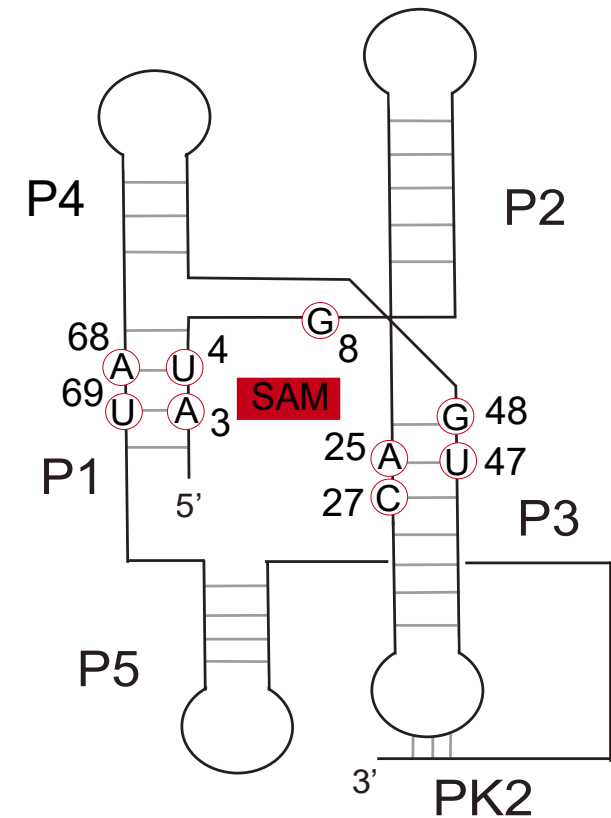
SAM-I



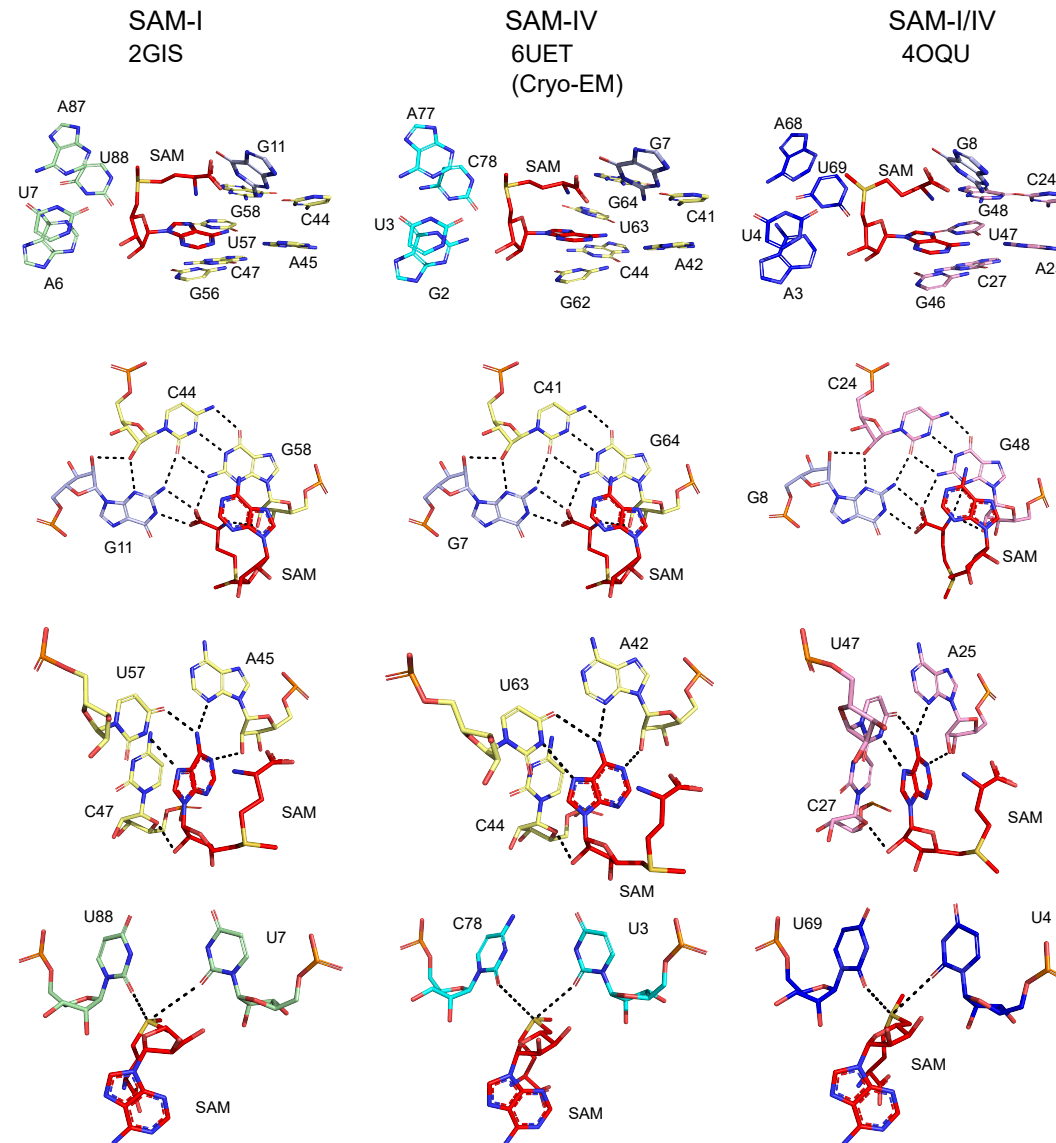
SAM-IV



SAM-I/IV



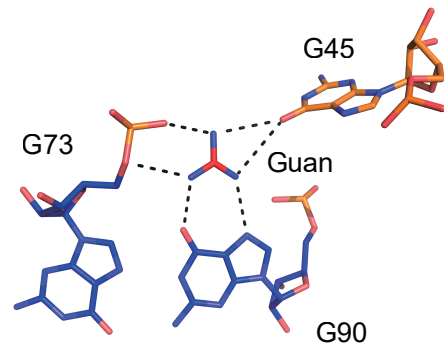
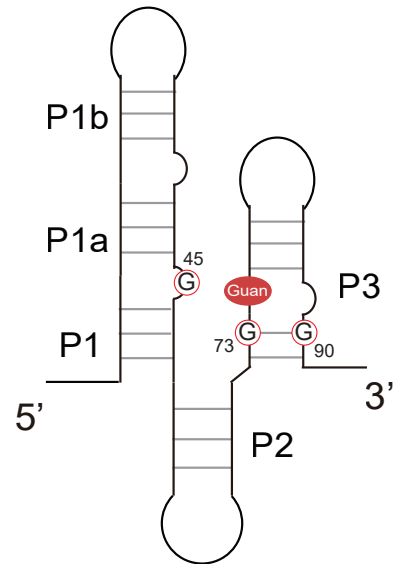
the binding pocket can be a local template!



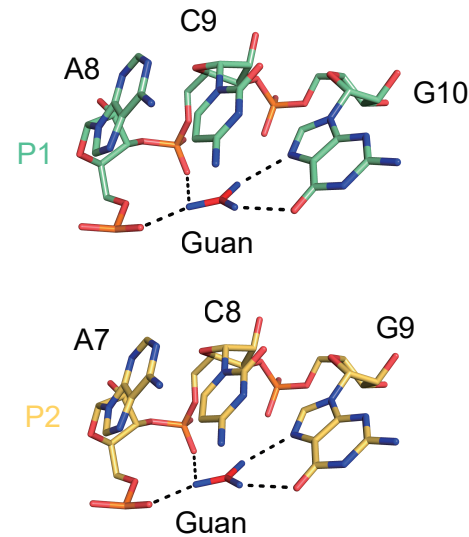
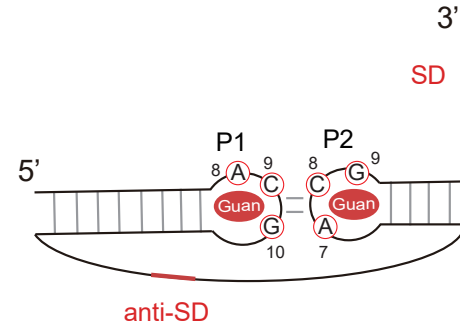
Binding pocket structural similarity



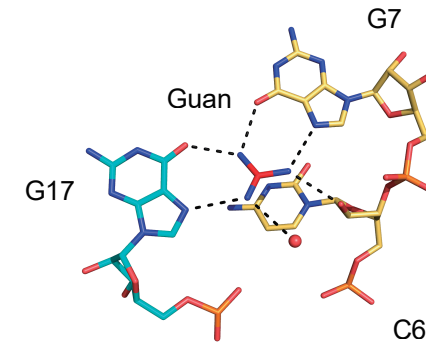
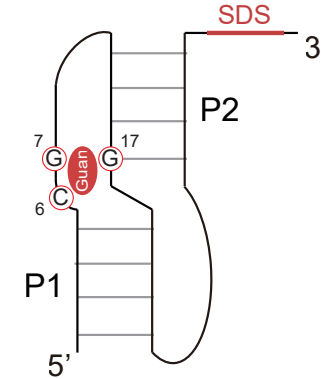
Guanidine-I



Guanidine-II



Guanidine-III



Best models across riboswitch puzzles

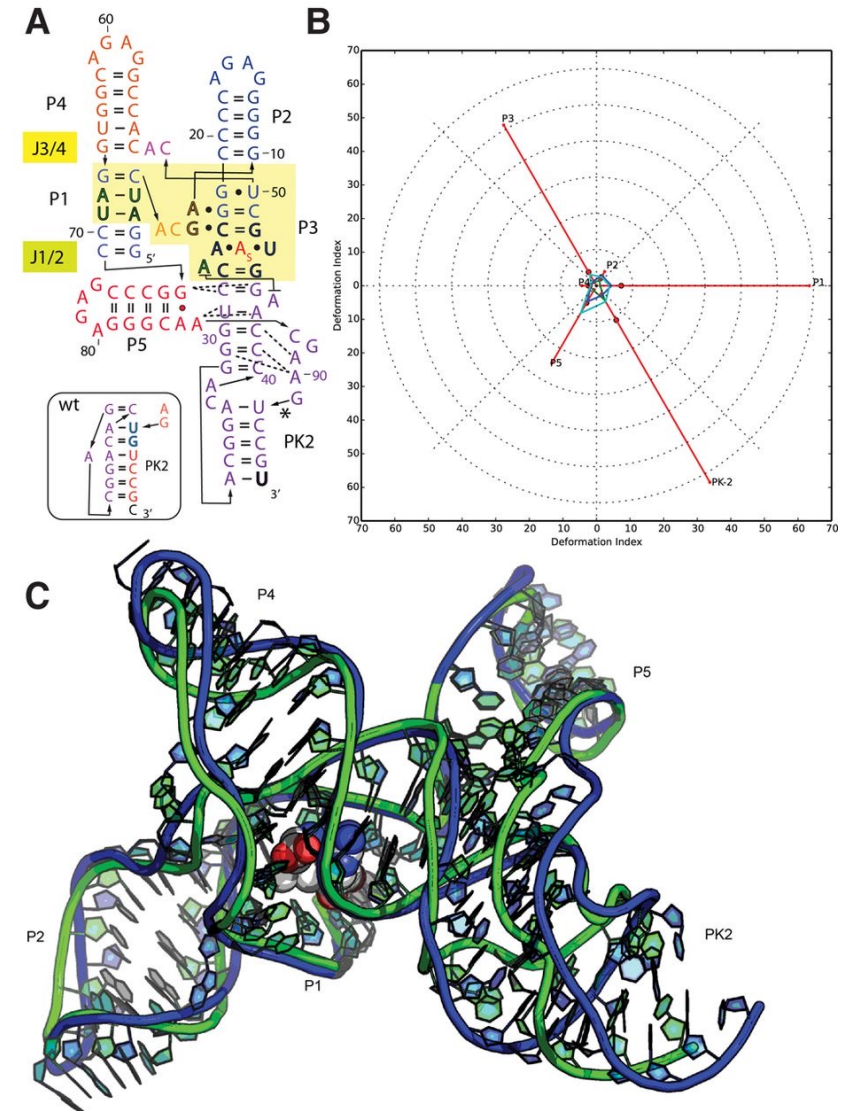
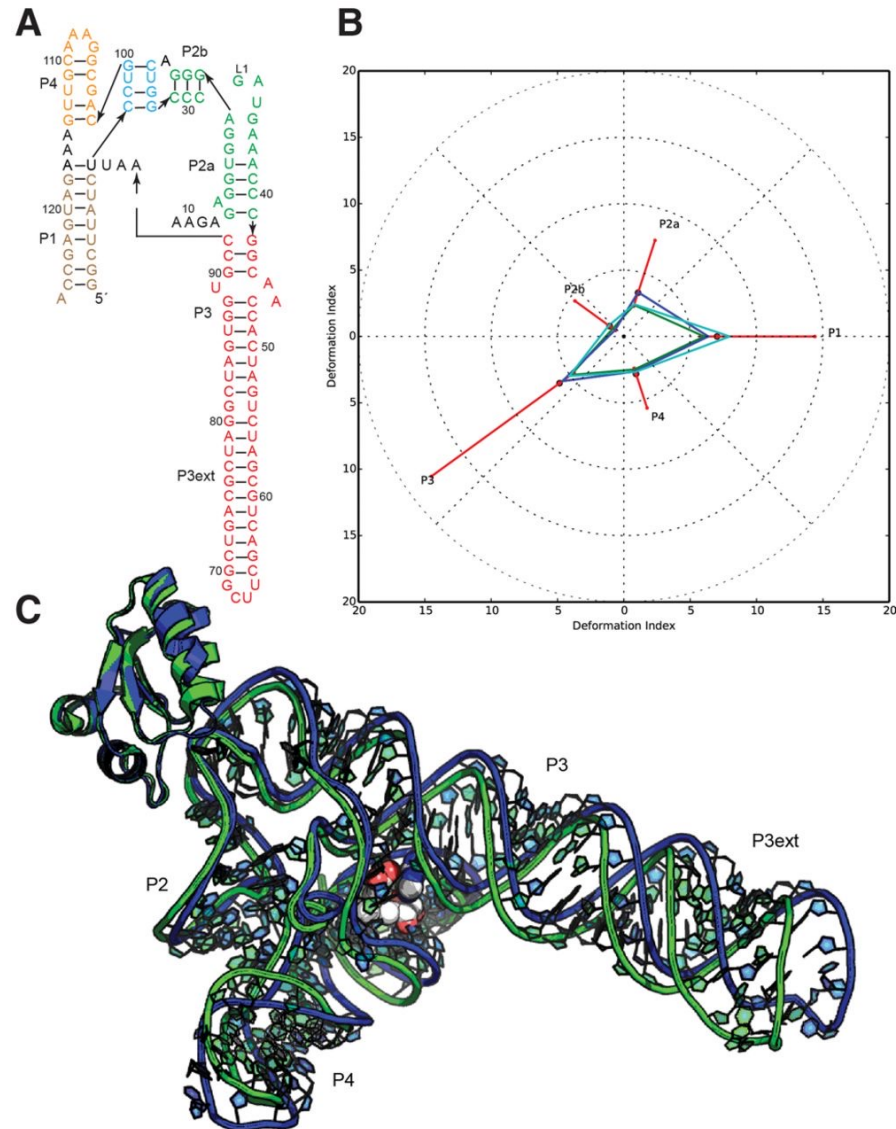


PZ	Riboswitch	Model	RMSD
3	Glycine	Chen 1	7.241
4	SAM-I aptamer	Chen 2	3.257
6	AdoCbl	Das 4	11.699
8	SAM-I/IV	Das 3	4.801
10	T-box tRNA	Das 3	6.803
12	ydaO c-di-AMP	Ding 12	10.061
13	ZMP	Das 7	5.410
14F	L-Gln free	Das PE 2	6.513
14B	L-Gln bound	Buj PE 2	4.994
17	Pistol	SimRNA 1	5.145
21	Guanidine III	Das LR 1	3.646

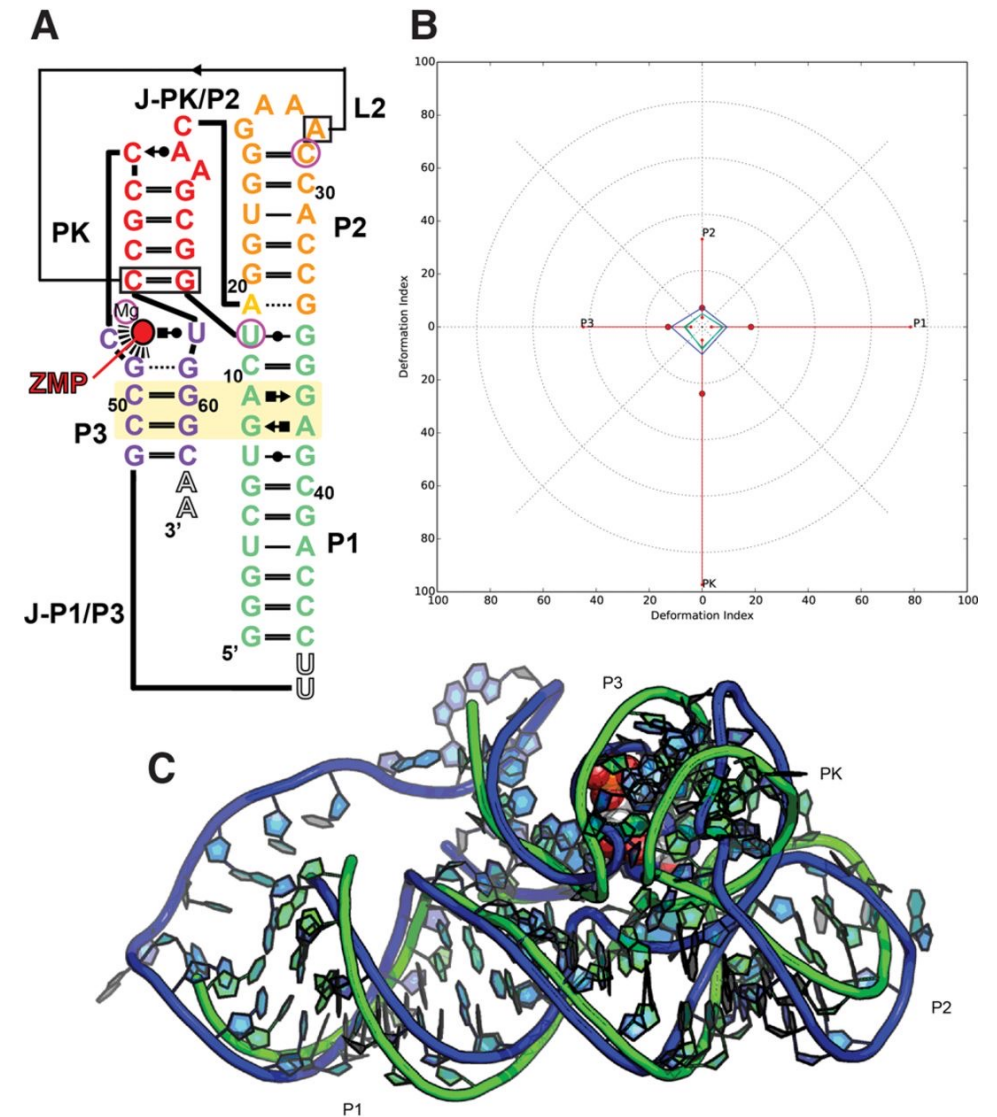
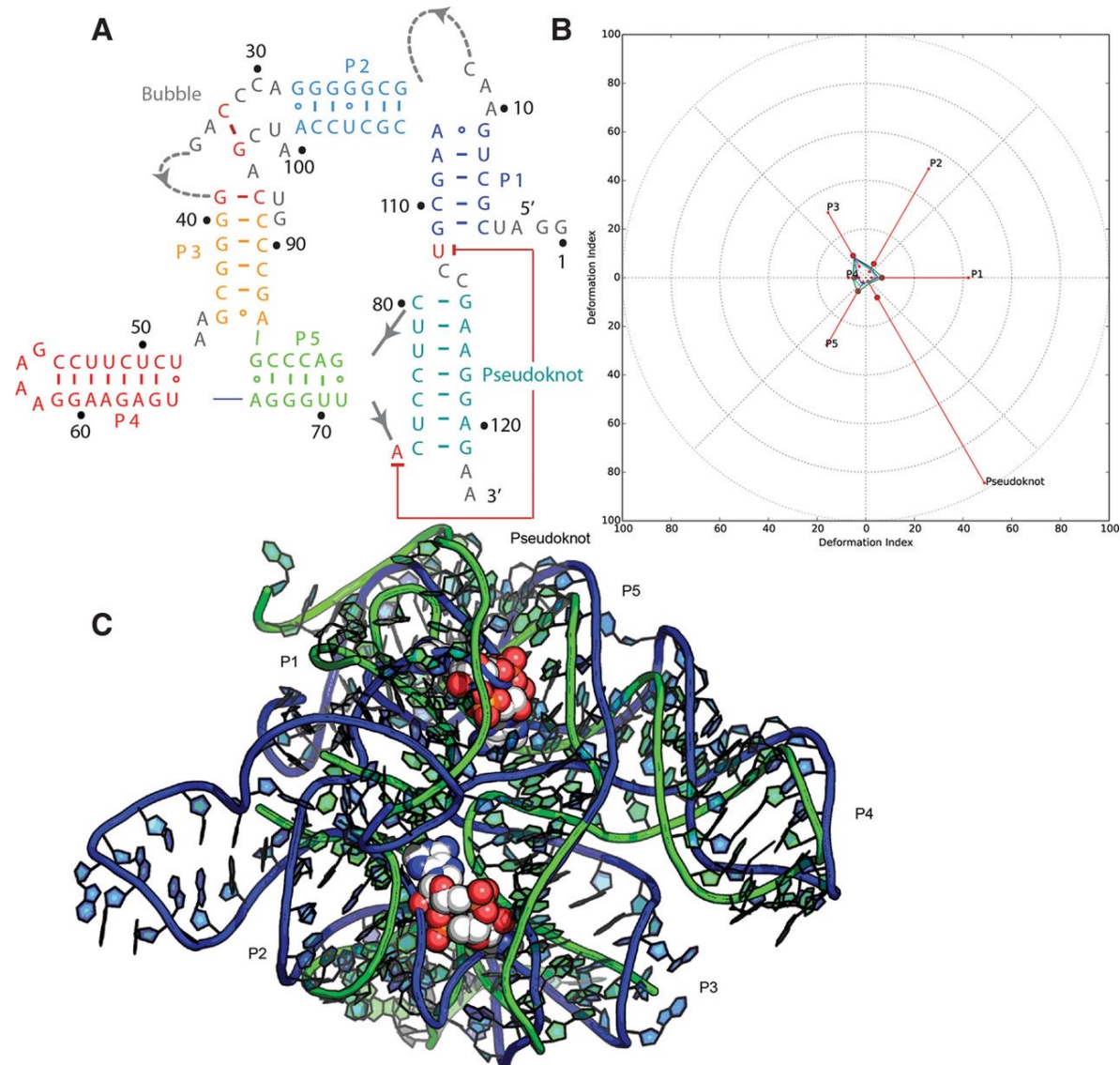
PZ	Riboswitch	Model	RMSD
25	2'-dG-II	Chen 5	2.551
26	T-box Gk glyQ	TFN 3	12.458
27	T-box Bs glyQS	TFN 2	9.498
28	T-box Nf ileS	TFN 3	14.504
29	NAD+	RNAComp 1	4.297
37	NAD+ II	Chen 6	5.420
38	NAD+ II alt	Chen 3	7.978
44	THF-II		
44	foIE		
47	2'-dG-III		

Best model = lowest RMSD in each result table. PZ 40-79 are intentionally blank.

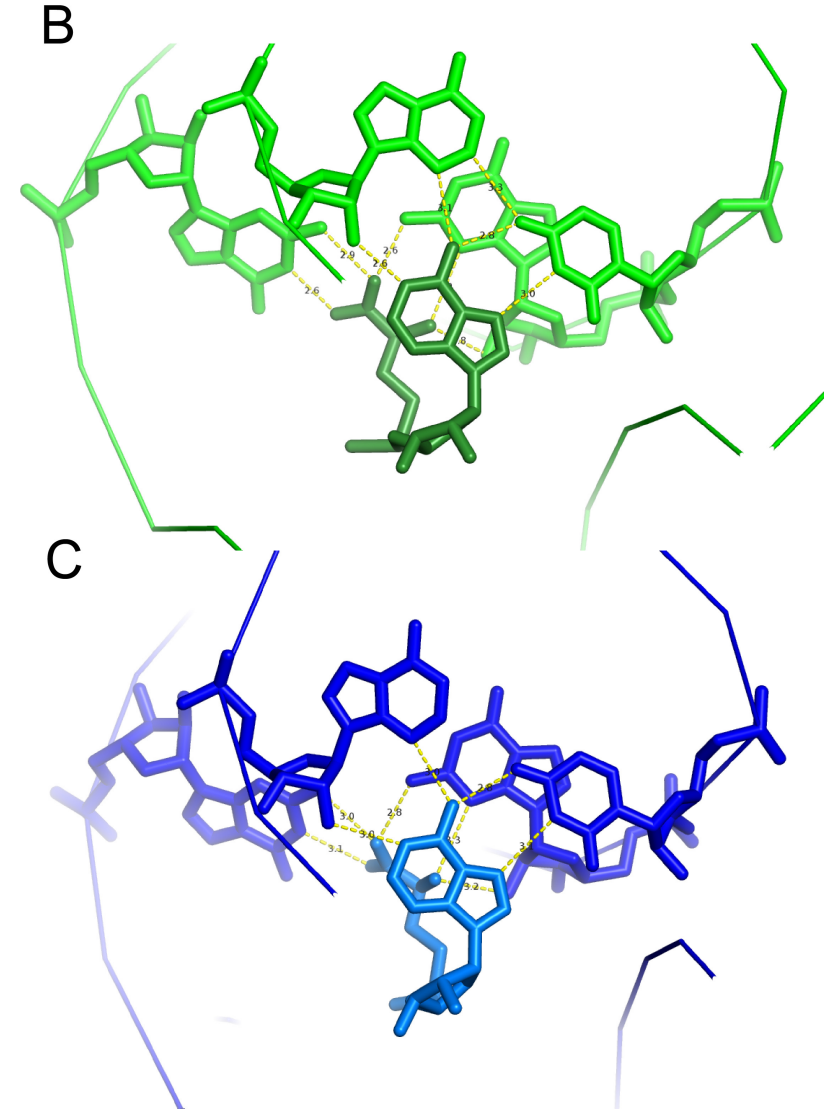
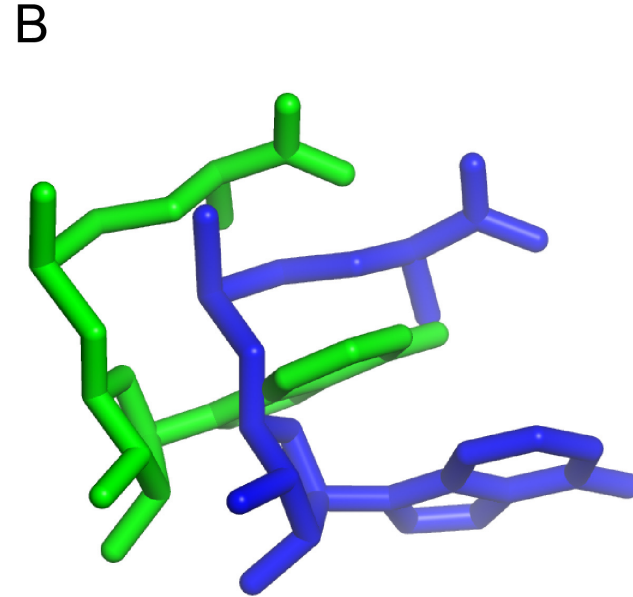
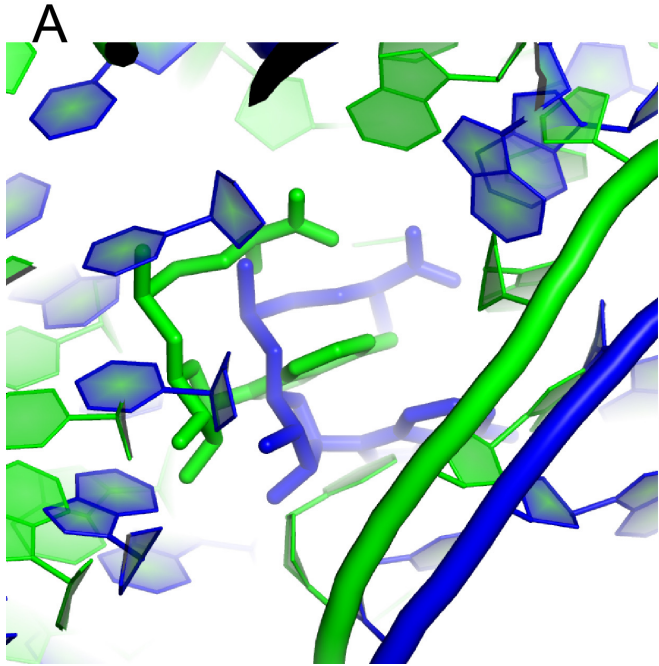
Cases in RNA-Puzzles



Cases in RNA-Puzzles



Binding pocket region in RNA-Puzzles





- **Ligand binding may show common mechanism in riboswitches**
- **Binding pockets show certain conservation**
- **Known binding pockets can be used as local template in 3D prediction**

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Acknowledgements



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