

Job summary

Job ID:	4gxy-demo
Date:	2026-05-11 21:13 UTC
Sequence length:	161 nt
Conformers:	5
Pockets detected:	45 (across all frames)
Clusters:	16 (12 passing persistence floor)
Top-3 surfaced:	3
RhoFold pLDDT (mean):	75.140

Sequence:

```
GCGGCAGGUGCUCGCCGACGUCGGGAGUUAAAAGGGAAGCCGGUGCAAGUCCGGCACGGUCCCGCCACUGUGACGGGGAGU  
CGCCCCUCGGGAUGUGCCACUGGCCCGCCGGGAAGGCGGAGGGCGGCGAGGAUCCGGAGUCAGGAAACCUGCCUGCCG  
U
```

Top-3 candidate druggable pockets

#1 Cluster 1 (geometric rank #1)

NEAR (35%)

Persistence:

1.00 (5 of 5 frames)

Geometric score (ranking):

12.000 = persistence × n_residues_intersected (1.00 × 12)

Mean druggability (metadata, not ranking):

0.001 -- fpocket protein-trained score, see Methods

Median druggability:

0.001

Max druggability:

0.001

Centroid (A):

6.47 -4.36 -6.53

Residues (union):

66, 67, 68, 99, 100, 101, 112, 113, 114, 145, 146, 147

Residues (intersection):

66, 67, 68, 99, 100, 101, 112, 113, 114, 145, 146, 147

Binding-site overlap (benchmark):

6/17 residues (35%) - near ($\geq 30\%$ of binding-site residues)

#2 Cluster 4 (geometric rank #2)

NEAR (35%)

Persistence:

1.00 (5 of 5 frames)

Geometric score (ranking):

9.000 = persistence × n_residues_intersected (1.00 × 9)

Mean druggability (metadata, not ranking):

0.004 -- fpocket protein-trained score, see Methods

Median druggability:

0.003

Max druggability:

0.009

Centroid (A):

1.28 4.42 2.72

Residues (union):

35, 36, 37, 65, 66, 67, 68, 69, 140, 141, 142, 143, 144, 145, 146

Residues (intersection):

66, 67, 68, 69, 140, 141, 142, 143, 144

Binding-site overlap (benchmark):

6/17 residues (35%) - near ($\geq 30\%$ of binding-site residues)

#3 Cluster 5 (geometric rank #3)

NONE (6%)

Persistence:

1.00 (5 of 5 frames)

Geometric score (ranking):

5.000 = persistence × n_residues_intersected (1.00 × 5)

Mean druggability (metadata, not ranking):

0.094 -- fpocket protein-trained score, see Methods

Median druggability:

0.066

Max druggability:

0.196

Centroid (A):

9.22 -10.53 -14.73

Residues (union):

95, 96, 97, 98, 112, 113, 114, 116, 117

Residues (intersection):

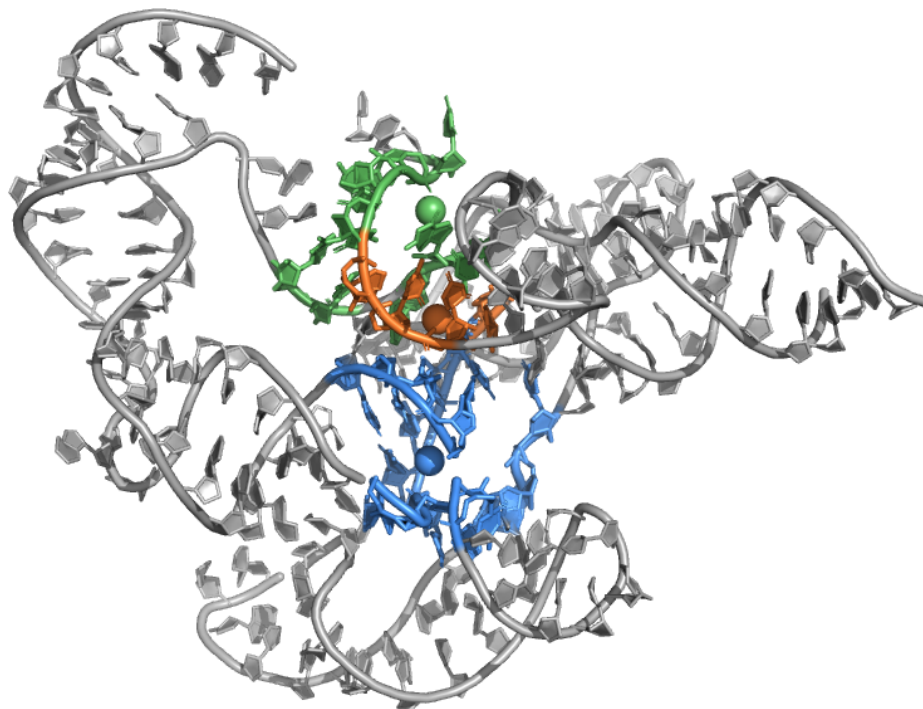
95, 96, 97, 112, 113

Binding-site overlap (benchmark):

1/17 residues (6%) - neither strict nor near

Predicted structure with top-3 pockets

Cartoon backbone, gray. Top-3 pocket residues highlighted (orange / azure / green = ranks 1 / 2 / 3). Centroid spheres shown at the geometric centre of each cluster's Kabsch-aligned member centres. Legend: #1 = cluster 1; #2 = cluster 4; #3 = cluster 5.



Methods

v0.2 ranks candidate pockets by structural persistence across the conformational ensemble, weighted by binding-residue stability (score = persistence x n_residues_intersected). This replaces the v0.1 ranker, which used fpocket's druggability score as the primary ranking signal. fpocket's druggability score is the output of a logistic regression trained on protein druggable-vs-non-druggable cavities; its dominant feature is normalised against a protein hydrophobic-density range that does not transfer to RNA cavities. On validated RNA benchmark targets the protein-trained classifier consistently scored the actual binding-site cluster near zero while assigning non-binding cavities scores in the 0.1-0.7 range. The geometric ranker recovers the binding-site cluster at rank-1 on 3 of 4 v0.1 retro benchmark targets vs 0 of 4 with the previous ranker. fpocket's druggability score is still computed and reported per cluster as metadata; druggability assessment itself is left to the customer's medicinal chemistry workflow.

Structures are predicted using RhoFold+ (Apache 2.0). Conformational ensemble generated by anisotropic network model (ANM) normal-mode sampling on the C3' backbone, perturbing along the 10 lowest-frequency collective modes (ProDy, BSD-3). Pockets detected per conformer using fpocket (MIT) with RNA-tuned alpha-sphere and clustering parameters (min radius 3.0 Å, max 5.7 Å, min alpha-spheres 35, clustering distance 1.65 Å). Pockets are clustered across the ensemble after Kabsch-aligning frames to the reference. Persistence is the fraction of frames a cluster is detected in; binding-residue stability is the count of residues contacted by the cluster in every member frame. Clusters with persistence below the configured floor are excluded from the customer-visible top-3.

For targets with diverse-tail evolutionary representation (sequences with at least one homolog at <77% identity, or a non-trivial fraction of homologs in the 70-80% identity band), an MSA-aware structure prediction path is available as an opt-in mode. This empirical screening criterion is calibrated on a benchmark of seven RNA targets and will be refined as more targets accumulate. Single-sequence prediction is the default for all other targets.

Results are computational predictions. Experimental validation is required before use in drug development or clinical applications.

Binding-mode caveat

Pipeline detects cleft-shaped binding pockets. Groove-binding modes and shallow surface-deformation binding may be missed. Contact us if your target's binding mode is groove-mediated.

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