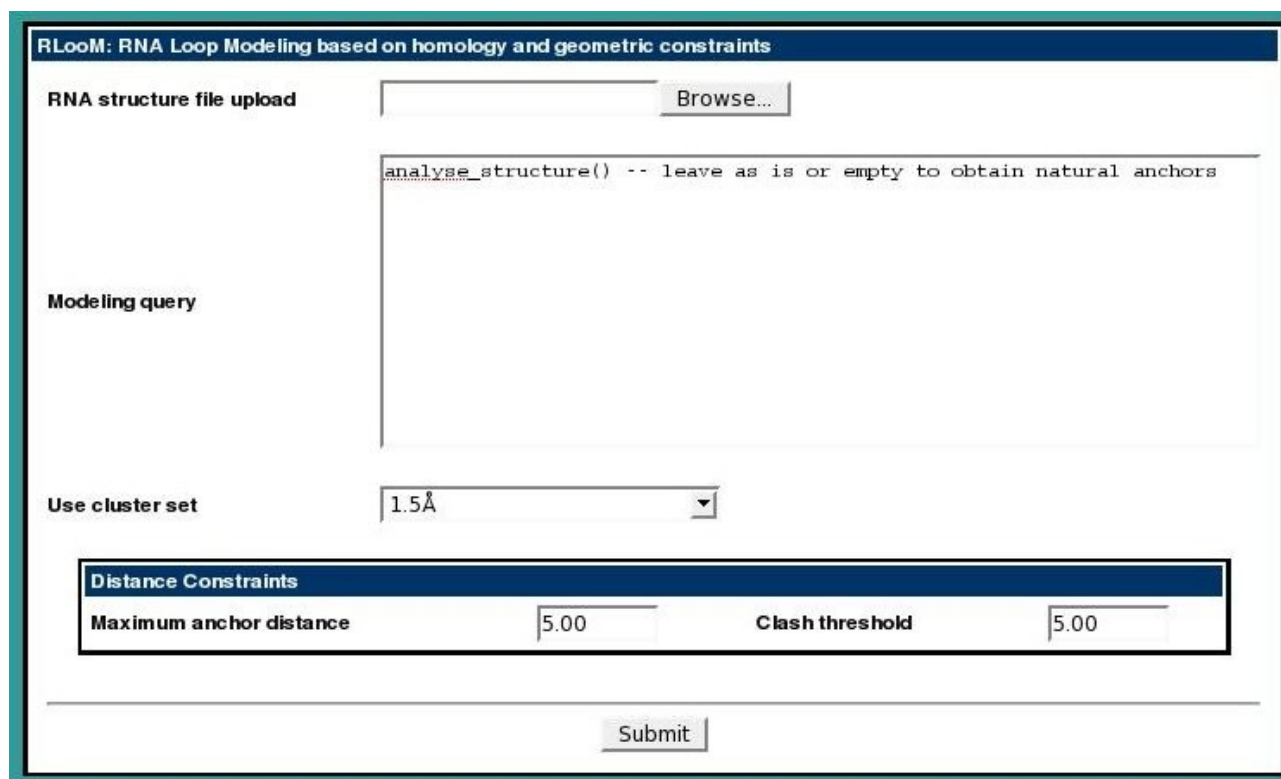**How to perform RNA loop modeling with RlooM?**
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In this tutorial, we will exchange a tRNA D-loop against a hairpin loop with a slightly modified sequence of the same length (10 bases.)

1. Download the target structure file from http://rloom.mpimp-golm.mpg.de/suppl/target1.pdb
2. The modeling tool is accessible from the RlooM homepage at http://rloom.mpimp-golm.mpg.de (left side "Model new loop") or directly from http://rloom.mpimp-golm.mpg.de/rloom.py.
3. You will now see the RLooM modeling interface (Figure 1.)
4. Use the **RNA structure file upload** field to select the target structure to be uploaded. Select the target file you downloaded in step 1.
5. The **Modeling query** field takes as input a list of commands in RLML (s. below or online help.) If you already know the anchors for the loop to be modeled, you can enter your RLML commands here. Otherwise, you can have RlooM analyse your target structure (command: analyse_structure()) and provide you a list of possible anchors as inferred from the secondary structure of the molecule.
    For this tutorial, leave the field as it is, so RlooM can detect the native anchors of the structure.
6. We leave the **Distance constraints** untouched for this tutorial. These parameters allow the user to decide at which atom-atom distance a loop does not fit into a target site (**Maximum anchor distance**) and when a clash occurs (**Clash treshold**.)
7. Click **Submit**, then wait for a moment while RlooM analyses the uploaded structure and searches for secondary structure elements and their anchors.

Figure 1: The RLooM modeling interface – structure upload.

When the analysis of the structure is complete, you will see a slightly different version of the RLooM modeling interface (Figure 2.) Please note, that the structure file upload field has been replaced by a list field, the **Select anchors** list. In this field, all found secondary structure elements are listed, together with their anchors. Internal loops and multiloops are listed together with all their constituting segments. Elements from the list can be selected (via double clicking) to be included in the loop modeling. A double-click-selection of an element, inserts a piece of RLML code, representing the selected element, into the **Modeling query** field. If the desired loop is not among the elements of the list, the user can also directly type the RLML code for their target into the **Modeling query** field, i.e. the modeling is not restricted to regions found by the secondary structure analysis.

8. To go on with the modeling, double click the hairpin loop located between bases 12:A and 23:A.
9. We will allow a number of mismatch in the templates: enter the query sequence for the loop, by inserting `<query k=3>UAAUGGUCAG</query>` somewhere within the `<hairpin>...</hairpin>` hierarchy (e.g. like in Figure 2.)
10. The **Use cluster set** field allows the user to set the template data set used for the modeling. Select the **0.5A with sequence identity** set.
11. Click **Submit**. The RLooM server will now start fitting all loops in the chosen template set that confirm to the query sequence, into the target site that we specified in step 8. The website will auto-refresh until the computations are done. If you don't want to wait, you can copy the model id string (or the current URL in your browser, if it already contains the model id) to return to the site and view the results at a later point in time. To return to the modeling the model id can be inserted into the **Fetch session** field at the left navigation bar.

Figure 2: The RLooM modeling interface -- anchor list and RLML

12. After a short while, the computations will be finished and the results page will be displayed (cf. Figure 3.) Here, you can obtain more information about the used templates (by clicking on the template ids), about the structural quality of the anchor fit, the edit distance of templates as compared to the query sequence etc. Additionally, you can view your uploaded structure with the attached template (if your browser supports Java) and download the model structure.

How to perform modeling of multiple RNA loops at once?

13. You will surely have noticed the "**I don't like these templates. Don't use any of them.**" option at the bottom of the list, as well as the **Merge** button. These input elements are used for multiple modeling sessions. A modeling script can be used to model four individual hairpins or segments simultaneously. In such a case, multiple result-lists will we displayed on the same page. The user can then use the radio buttons on the left side of the list to choose a template for each loop (or use the "**I don't like these templates. Don't use any of them.**" option to ignore the respective loop) and then create a model containing all attached templates using the **Merge** button. This model will then be directly offered for download.

Loop 0							
	Cluster (Structure)	Sequence	RMSD$_a$ [Å]	Δedit (k)	Clash?	View	Download
○	Hairpin 010:207 (2tra:A, 12-23)	UAAUGGUCAG	0.000	0	False	Jmol	PDB
○	Hairpin 010:263 (3tra:A, 12-23)	UAAUGGUCAG	0.159	0	True	Jmol	PDB
○	Hairpin 010:3 (1asz:S, 12-23)	UAAUGGUCAG	0.279	0	True	Jmol	PDB
○	Hairpin 010:1 (1asy:S, 12-23)	UAAUGGUCAG	0.308	0	True	Jmol	PDB
○	Hairpin 010:0 (1asy:R, 12-23)	UAAUGGUCAG	0.418	0	True	Jmol	PDB
○	Hairpin 010:17 (1f7v:B, 12-23)	CAAUGGUCAC	0.448	2	True	Jmol	PDB
○	Hairpin 010:16 (1f7u:B, 12-23)	CAAUGGUCAC	0.452	2	True	Jmol	PDB
○	Hairpin 010:32 (1i2:C, 12-23)	UAAUGGUCAG	0.465	0	True	Jmol	PDB
○	Hairpin 010:33 (1i2:D, 11-22)	UAAUGGUCAG	0.509	0	True	Jmol	PDB
○	Hairpin 010:152 (2d6f:F, 12-23)	UAGUGGUAAU	0.903	3	True	Jmol	PDB
○	**I don't like these templates. Don't use any of them.**						
	Merge						

Figure 3: The RLooM results page