

Summary of integrative structure determination of Hybrid NMR-SAXS structure of a trans-cleaving VS ribozyme (PDB ID: 9A0V, PDB-Dev ID: PDBDEV_00000067)

1. Model Composition	
<i>Entry composition</i>	Neurospora Varkud Satellite Ribozyme: chain(s) A (101 residues)
<i>Datasets used for modeling</i>	<ul style="list-style-type: none"> - NMR data, BMRB: 25654 - NMR data, BMRB: 25163 - NMR data, BMRB: 17292 - NMR data, BMRB: 50637 - SAS data, SASBDB: SASDKU3 - SAS data, SASBDB: SASDKV3 - SAS data, SASBDB: SASDKW3 - SAS data, SASBDB: SASDKY3 - Experimental model, PDB: 2N3Q - Experimental model, PDB: 2MTJ - Experimental model, PDB: 2L5Z - Experimental model, PDB: 1YN1
2. Representation	
<i>Number of representations</i>	1
<i>Scale</i>	Atomic
<i>Number of rigid and flexible segments</i>	0, 15
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	<ul style="list-style-type: none"> - 4 unique SASRestraint: Assembly name: Complete assembly Fitting method: Crysol Multi-state: False
4. Validation	
<i>Number of ensembles</i>	0
<i>Number of models in ensembles</i>	Not applicable
<i>Number of deposited models</i>	10
<i>Model precision (uncertainty of models)</i>	Not available
<i>Data quality</i>	
<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 0.62-0.62 - Ramachandran outliers: 0-0 - Sidechain outliers: 0-0

<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <u>Name</u>	?
<u>Method</u>	fragment assembly
<u>Description</u>	?
<u>Number of computed models</u>	?
2. <u>Name</u>	?
<u>Method</u>	refinement
<u>Description</u>	?
<u>Number of computed models</u>	?
<u>Software</u>	<ul style="list-style-type: none"> - ORNAS (version Not available) - Pymol (version Not available) - Crysol (version Not available)