

**Summary of integrative structure determination of Integrative Modeling  
of a Sin3/HDAC Complex Sub-structure (PDB ID: 9A07, PDB-Dev ID:  
PDBDEV\_00000043)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- SAP30L C terminal: chain(s) A (90 residues)</li> <li>- SAP30L N terminal: chain(s) B (68 residues)</li> <li>- SIN3A: chain(s) C (122 residues)</li> <li>- HDAC1: chain(s) D (369 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Comparative model, Not available</li> <li>- Comparative model, Not available</li> <li>- Comparative model, Not available</li> <li>- Comparative model, Not available</li> <li>- Crosslinking-MS data, MASSIVE: <a href="#">MSV000084311</a></li> <li>- Experimental model, PDB: <a href="#">2LD7</a></li> <li>- Experimental model, PDB: <a href="#">2N1U</a></li> <li>- Experimental model, PDB: <a href="#">2N2H</a></li> <li>- Experimental model, PDB: <a href="#">5IX0</a></li> <li>- Mutagenesis data, Not available: <a href="#">10.1074/jbc.RA119.009780</a></li> </ul>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Atomic
Number of <a href="#">rigid</a> and <a href="#">flexible</a> segments	4, 0
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	<ul style="list-style-type: none"> <li>- 1 unique CrossLinkRestraint: DSSO, 12 crosslinks</li> <li>- 16 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0</li> </ul>
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	0
<a href="#">Number of models in ensembles</a>	Not applicable
<a href="#">Number of deposited models</a>	1
<a href="#">Model precision (uncertainty of models)</a>	Not available
<a href="#">Data quality</a>	Data quality has not been assessed

<a href="#"><i>Model quality: assessment of atomic segments</i></a>	<ul style="list-style-type: none"> <li>- Clashscore: 5.99</li> <li>- Ramachandran outliers: 3</li> <li>- Sidechain outliers: 46</li> </ul>
<a href="#"><i>Fit to data used for modeling</i></a>	Satisfaction of crosslinks: 100.00%
<a href="#"><i>Fit to data used for validation</i></a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#"><i>Name</i></a>	?
<a href="#"><i>Method</i></a>	comparative modeling
<a href="#"><i>Number of computed models</i></a>	?
2. <a href="#"><i>Name</i></a>	?
<a href="#"><i>Method</i></a>	docking
<a href="#"><i>Number of computed models</i></a>	200
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"> <li>- <a href="#">HADDOCK</a> (version Not available)</li> <li>- <a href="#">SWISS-MODEL</a> (version Not available)</li> </ul>