

**Summary of integrative structure determination of Integrative model of full-length RAGE in complex with S100B (PDB ID: 9A18, PDB-Dev ID: PDBDEV\_00000080)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- RAGE: chain(s) A, B, C, D (383 residues)</li> <li>- S100B: chain(s) E, F, G, H (91 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Experimental model, PDB: <a href="#">4ybh</a></li> <li>- Experimental model, PDB: <a href="#">4xyn</a></li> <li>- Experimental model, PDB: <a href="#">5d7f</a></li> <li>- Crosslinking-MS data, MASSIVE: <a href="#">MSV000086438</a></li> <li>- Crosslinking-MS data, MASSIVE: <a href="#">MSV000086437</a></li> <li>- H/D exchange data, MASSIVE: <a href="#">MSV000086718</a></li> </ul>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Atomic
<a href="#">Number of <i>rigid</i> and <i>flexible</i> segments</a>	0, 12
<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: BS3, 27 crosslinks</li> <li>- 1 unique CrossLinkRestraint: BS3, 39 crosslinks</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="#">Model quality: assessment of atomic segments</a>	<ul style="list-style-type: none"> <li>- Clashscore: 16.39</li> <li>- Ramachandran outliers: 15</li> <li>- Sidechain outliers: 6</li> </ul>
<a href="#">Fit to data used for modeling</a>	Satisfaction of crosslinks: 92.42%

<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>	modeling
<a href="#"><i>Method</i></a>	?
<a href="#"><i>Description</i></a>	?
<a href="#"><i>Number of computed models</i></a>	?
<a href="#"><i>Software</i></a>	<a href="#">ROSETTA</a> (version Not available)