

**Summary of integrative structure determination of Integrative threading of the DNA-PKcs sequence based on data from chemical cross-linking and hydrogen deuterium exchange (PDB ID: 8ZZY, PDB-Dev ID: PDBDEV\_00000034)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	DNA-PKcs: Chain A (4128 residues)
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Crosslinking-MS data, Linker name and number of cross-links: DSG, 63 cross-links</li> <li>- Crosslinking-MS data, Linker name and number of cross-links: DSS, 48 cross-links</li> <li>- Crosslinking-MS data, Linker name and number of cross-links: BSP, 52 cross-links</li> <li>- H/D exchange data, PRIDE: PXD016595</li> <li>- Experimental model, PDB ID: 5LUQ</li> </ul>
<b>2. Representation</b>	
<a href="#">Resolution</a>	Coarse-grained: 1 residue(s) per bead
<a href="#">Number of rigid bodies, flexible units</a>	1, 0
<a href="#">Rigid bodies</a>	A: 1-4128
<a href="#">Structural coverage (rigid bodies)</a>	100%
<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: DSG, 63 cross-links</li> <li>- 1 unique CrossLinkRestraint: DSS, 48 cross-links</li> <li>- 1 unique CrossLinkRestraint: BSP, 52 cross-links</li> </ul>
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	2
<a href="#">Number of models in ensembles</a>	2758, 2242
<a href="#">Number of deposited models</a>	10
<a href="#">Model precision (uncertainty of models)</a>	None, Å, None, Å
<a href="#">Data quality</a>	Data quality has not been assessed
<a href="#">Model quality: assessment of excluded volume</a>	Satisfaction: 100.00-100.00%
<a href="#">Fit to data used for modeling</a>	Fit of model to information used to compute it has not been determined

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<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>Method</i></a>	Production sampling
<a href="#"><i>Name</i></a>	Enumeration
<a href="#"><i>Number of computed models</i></a>	2860000
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"><li>- <a href="#">PSIPRED</a> (version 4.0)</li><li>- <a href="#">Integrative Modeling Platform (IMP)</a> (version 2.2)</li><li>- <a href="#">scikit-learn</a> (version 0.21.3)</li></ul>