

**Summary of integrative structure determination of Modeling of the interaction between doublecortin and microtubule, NDCs fixed at lateral orientation (PDB ID: 9A10, PDB-Dev ID: PDBDEV\_0000072)**

<b>1. Model Composition</b>	
<p><a href="#">Entry composition</a></p>	<ul style="list-style-type: none"> <li>- Beta-Tubulin: Chain Q (445 residues)</li> <li>- Beta-Tubulin: Chain S (445 residues)</li> <li>- Beta-Tubulin: Chain T (445 residues)</li> <li>- Alpha-Tubulin: Chain H (451 residues)</li> <li>- Alpha-Tubulin: Chain E (451 residues)</li> <li>- Alpha-Tubulin: Chain L (451 residues)</li> <li>- Beta-Tubulin: Chain U (445 residues)</li> <li>- Doublecortin: Chain A (365 residues)</li> <li>- Beta-Tubulin: Chain X (445 residues)</li> <li>- Beta-Tubulin: Chain P (445 residues)</li> <li>- Beta-Tubulin: Chain W (445 residues)</li> <li>- Beta-Tubulin: Chain Z (445 residues)</li> <li>- Doublecortin: Chain B (365 residues)</li> <li>- Beta-Tubulin: Chain V (445 residues)</li> <li>- Beta-Tubulin: Chain Y (445 residues)</li> <li>- Beta-Tubulin: Chain R (445 residues)</li> <li>- Alpha-Tubulin: Chain K (451 residues)</li> <li>- Alpha-Tubulin: Chain M (451 residues)</li> <li>- Beta-Tubulin: Chain O (445 residues)</li> <li>- Alpha-Tubulin: Chain I (451 residues)</li> <li>- Alpha-Tubulin: Chain F (451 residues)</li> <li>- Alpha-Tubulin: Chain C (451 residues)</li> <li>- Alpha-Tubulin: Chain G (451 residues)</li> <li>- Alpha-Tubulin: Chain J (451 residues)</li> <li>- Alpha-Tubulin: Chain D (451 residues)</li> <li>- Alpha-Tubulin: Chain N (451 residues)</li> </ul>
<p><a href="#">Datasets used for modeling</a></p>	<ul style="list-style-type: none"> <li>- Experimental model, PDB ID: 4ATU</li> <li>- Experimental model, PDB ID: 6FNZ</li> <li>- Experimental model, PDB ID: 6EVZ</li> <li>- Crosslinking-MS data, Linker name and number of cross-links: LCSDA, 445 cross-links</li> </ul>
<b>2. Representation</b>	
<p><a href="#">Resolution</a></p>	<p>Coarse-grained: 1, 4, 8 residue(s) per bead</p>
<p>Number of <a href="#">rigid bodies</a>, <a href="#">flexible units</a></p>	<p>52, 4</p>

<i>Rigid bodies</i>	<ul style="list-style-type: none"> <li>- A: 51-140, 177-251</li> <li>- B: 51-140, 177-251</li> <li>- C: 1-37, 47-435</li> <li>- D: 1-37, 47-435</li> <li>- E: 1-37, 47-435</li> <li>- F: 1-37, 47-435</li> <li>- G: 1-37, 47-435</li> <li>- H: 1-37, 47-435</li> <li>- I: 1-37, 47-435</li> <li>- J: 1-37, 47-435</li> <li>- K: 1-37, 47-435</li> <li>- L: 1-37, 47-435</li> <li>- M: 1-37, 47-435</li> <li>- N: 1-37, 47-435</li> <li>- O: 1-37, 38-429</li> <li>- P: 1-37, 38-429</li> <li>- Q: 1-37, 38-429</li> <li>- R: 1-37, 38-429</li> <li>- S: 1-37, 38-429</li> <li>- T: 1-37, 38-429</li> <li>- U: 1-37, 38-429</li> <li>- V: 1-37, 38-429</li> <li>- W: 1-37, 38-429</li> <li>- X: 1-37, 38-429</li> <li>- Y: 1-37, 38-429</li> <li>- Z: 1-37, 38-429</li> </ul>
<i>Flexible units</i>	<ul style="list-style-type: none"> <li>- A: 141-176, 252-330</li> <li>- B: 141-176, 252-330</li> <li>- C: -</li> <li>- D: -</li> <li>- E: -</li> <li>- F: -</li> <li>- G: -</li> <li>- H: -</li> <li>- I: -</li> <li>- J: -</li> <li>- K: -</li> <li>- L: -</li> <li>- M: -</li> <li>- N: -</li> <li>- O: -</li> <li>- P: -</li> <li>- Q: -</li> <li>- R: -</li> <li>- S: -</li> <li>- T: -</li> <li>- U: -</li> <li>- V: -</li> <li>- W: -</li> <li>- X: -</li> <li>- Y: -</li> <li>- Z: -</li> </ul>
<u>Structural coverage (rigid bodies)</u>	98%
<b>3. Restraints</b>	
<u>Physical principles</u>	Information about physical principles was not provided

<a href="#">Experimental data</a>	- 1 unique CrossLinkRestraint: LCSDA, 445 cross-links
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	1
<a href="#">Number of models in ensembles</a>	30000
<a href="#">Number of deposited models</a>	1
<a href="#">Model precision (uncertainty of models)</a>	None, Å
<a href="#">Data quality</a>	Data quality has not been assessed
<a href="#">Model quality: assessment of excluded volume</a>	Satisfaction: 99.96-99.96%
<a href="#">Fit to data used for modeling</a>	Fit of model to information used to compute it has not been determined
<a href="#">Fit to data used for validation</a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#">Method</a>	Sampling
<a href="#">Name</a>	Replica exchange monte carlo
<a href="#">Number of computed models</a>	240000
<a href="#">Software</a>	- <a href="#">IMP PMI module</a> (version 2.14.0) - <a href="#">Integrative Modeling Platform (IMP)</a> (version 2.14.0)