

**Summary of integrative structure determination of Modeling of the interaction between doublecortin and microtubule, NDCs fixed at diagonal (#1) orientation (PDB ID: 9A0Z, PDB-Dev ID: PDBDEV\_0000071)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- Beta-Tubulin: Chain L (445 residues)</li> <li>- Doublecortin: Chain A (365 residues)</li> <li>- Beta-Tubulin: Chain M (445 residues)</li> <li>- Alpha-Tubulin: Chain F (451 residues)</li> <li>- Beta-Tubulin: Chain N (445 residues)</li> <li>- Alpha-Tubulin: Chain D (451 residues)</li> <li>- Beta-Tubulin: Chain O (445 residues)</li> <li>- Alpha-Tubulin: Chain G (451 residues)</li> <li>- Beta-Tubulin: Chain S (445 residues)</li> <li>- Doublecortin: Chain B (365 residues)</li> <li>- Alpha-Tubulin: Chain C (451 residues)</li> <li>- Beta-Tubulin: Chain R (445 residues)</li> <li>- Beta-Tubulin: Chain P (445 residues)</li> <li>- Alpha-Tubulin: Chain K (451 residues)</li> <li>- Alpha-Tubulin: Chain H (451 residues)</li> <li>- Alpha-Tubulin: Chain I (451 residues)</li> <li>- Beta-Tubulin: Chain T (445 residues)</li> <li>- Alpha-Tubulin: Chain J (451 residues)</li> <li>- Beta-Tubulin: Chain Q (445 residues)</li> <li>- Alpha-Tubulin: Chain E (451 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<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>	
<a href="#">Resolution</a>	Coarse-grained: 1, 4, 8 residue(s) per bead
<a href="#">Number of <i>rigid bodies</i>, <i>flexible units</i></a>	40, 4
<a href="#">Rigid bodies</a>	<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, 38-429</li> <li>- M: 1-37, 38-429</li> <li>- N: 1-37, 38-429</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> </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> </ul>
<i>Structural coverage (rigid bodies)</i>	97%
<b>3. Restraints</b>	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	- 1 unique CrossLinkRestraint: LCSDA, 445 cross-links
<b>4. Validation</b>	
<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	30000
<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	None, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.94-99.94%
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
<i>1. Method</i>	Sampling
<i>Name</i>	Replica exchange monte carlo

---

<u><a href="#">Number of computed models</a></u>	240000
<u><a href="#">Software</a></u>	- <u><a href="#">IMP PMI module</a></u> (version 2.14.0) - <u><a href="#">Integrative Modeling Platform (IMP)</a></u> (version 2.14.0)