

Summary of integrative structure determination of Modeling of the interaction between doublecortin and microtubule, NDCs fixed at diagonal (#2) orientation (PDB ID: 9A12, PDB-Dev ID: PDBDEV_00000074)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Doublecortin: chain(s) A, B (365 residues) - Alpha-Tubulin: chain(s) C, D, E, F, G, H, I, J, K (451 residues) - Beta-Tubulin: chain(s) L, M, N, O, P, Q, R, S, T (445 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 4ATU - Experimental model, PDB: 6FNZ - Experimental model, PDB: 6EVZ - Crosslinking-MS data, Zenodo: 10.5281/zenodo.4526498
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
Number of <i>rigid</i> and <i>flexible</i> segments	40, 4
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: LCSDA, 445 crosslinks
4. Validation	
Number of ensembles	1
Number of models in ensembles	30000
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.94%
Fit to data used for modeling	Satisfaction of crosslinks: 35.51%
Fit to data used for validation	Fit of model to information not used to compute it has not been determined

5. Methodology and Software	
1. <i>Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	240000
<i>Software</i>	<ul style="list-style-type: none">- IMP PMI module (version 2.14.0)- Integrative Modeling Platform (IMP) (version 2.14.0)