

Summary of integrative structure determination of Modeling of the interaction between doublecortin and microtubule, NDCs fixed at longitudinal orientation (PDB ID: 9A11, PDB-Dev ID: PDBDEV_00000073)

| 1. Model Composition | |
|---|---|
| Entry composition | <ul style="list-style-type: none"> - Doublecortin: chain(s) A, B (365 residues) - Alpha-Tubulin: chain(s) C, D, G, H, I, J, K, L, M, N, O (451 residues) - Alpha-Tubulin: chain(s) E (451 residues) - Alpha-Tubulin: chain(s) F (451 residues) - Beta-Tubulin: chain(s) P, Q, R, S, T, U, V, W, X, Y, Z, AA (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 rigid and flexible segments | 52, 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: 99.96% |
| Fit to data used for modeling | Satisfaction of crosslinks: 30.19% |

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| <i>Fit to data used for validation</i> | 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) |