

Summary of integrative structure determination of Integrative structure of Smc5/6 complex (PDB ID: 9A19, PDB-Dev ID: PDBDEV_00000081)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - smc5: chain(s) A (1093 residues) - smc6: chain(s) B (1114 residues) - nse2: chain(s) C (267 residues) - nse5: chain(s) D (556 residues) - nse6: chain(s) E (464 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 6QPW - Experimental model, PDB: 6ZZ6 - Comparative model, Zenodo: 10.5281/zenodo.4685414 - Comparative model, Zenodo: 10.5281/zenodo.4685414 - Comparative model, Zenodo: 10.5281/zenodo.4685414 - Experimental model, PDB: 3HTK - Comparative model, Zenodo: 10.5281/zenodo.4685414 - Comparative model, Zenodo: 10.5281/zenodo.4685414 - Experimental model, PDB: 5MG8 - Comparative model, Zenodo: 10.5281/zenodo.4685414 - Comparative model, Zenodo: 10.5281/zenodo.4685414 - Comparative model, Zenodo: 10.5281/zenodo.4685414 - Comparative model, Zenodo: 10.5281/zenodo.4685414 - Comparative model, Zenodo: 10.5281/zenodo.4685414 - Comparative model, Zenodo: 10.5281/zenodo.4685414 - Experimental model, PDB: 7LTO - Experimental model, Zenodo: 10.5281/zenodo.4685414 - Mass Spectrometry data, PRIDE: PXD023164 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.4685414 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.4685414 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.4685414
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 115 residue(s) per bead
Number of rigid and flexible segments	35, 37
3. Restraints	

<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSSO, 159 crosslinks - 1 unique CrossLinkRestraint: DSSO, 109 crosslinks - 1 unique CrossLinkRestraint: CDI, 67 crosslinks
4. Validation	
<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	29975
<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	38.97, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.80%
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 92.19%
<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>	20000
2. <i>Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	100000
<i>Software</i>	<ul style="list-style-type: none"> - IMP PMI module (version develop-31a0ad09b4) - Integrative Modeling Platform (IMP) (version develop-31a0ad09b4) - MODELLER (version 9.25) - SWISS-MODEL (version 3.0.0)