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	- nse5: Chain D (556 residues) - nse6: Chain E (464 residues) - smc5: Chain A (1093 residues) - smc6: Chain B (1114 residues) - nse2: Chain C (267 residues)
Datasets used for modeling	- Experimental model, PDB ID: 6QPW - Experimental model, PDB ID: 6ZZ6 - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 3HTK - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 5MG8 - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 7LTO - Experimental model, PDB ID: Not available - Mass Spectrometry data, PRIDE: PXD023164 - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 159 cross-links - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 109 cross-links - Crosslinking-MS data, Linker name and number of cross-links: CDI, 67 cross-links
2. Representation	
Resolution	Coarse-grained: 1, 2, 3, 4, 10 residue(s) per bead
Number of rigid bodies, flexible units	35, 37

Rigid bodies	- A: 42-204, 208-266, 272-302, 304-363, 365-388, 398-459, 485-633, 653-676, 696-714, 719-737, 739-811, 851-880, 885-946, 950-1093 - B: 80-232, 236-294, 298-310, 314-430, 436-501, 506-692, 699-760, 770-882, 897-916, 923-939, 951-984, 988-1114 - C: 5-258 - D: 22-142, 185-257, 274-441 - E: 195-226, 238-379, 387-427, 431-441, 447-464
Flexible units	- A: 1-41, 205-207, 267-271, 303-303, 364-364, 389-397, 460-484, 634-652, 677-695, 715-718, 738-738, 812-850, 881-884, 947-949 - B: 1-79, 233-235, 295-297, 311-313, 431-435, 502-505, 693-698, 761-769, 883-896, 917-922, 940-950, 985-987 - C: 1-4, 259-267 - D: 1-21, 143-184, 258-273, 442-556 - E: 1-194, 227-237, 380-386, 428-430, 442-446
Structural coverage (rigid bodies)	79%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSSO, 159 cross-links - 1 unique CrossLinkRestraint: DSSO, 109 cross-links - 1 unique CrossLinkRestraint: CDI, 67 cross-links
4. Validation	
Number of ensembles	1
Number of models in ensembles	29975
Number of deposited models	1
Model precision (uncertainty of models)	38.97, Å
Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.80-99.80%
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
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. *Method*	Sampling

Name	Replica exchange monte carlo
Number of computed models	20000
2. Method	Sampling
Name	Replica exchange monte carlo
Number of computed models	100000
Software	- IMP PMI module (version develop-31a0ad09b4) - Integrative Modeling Platform (IMP) (version develop-31a0ad09b4) - MODELLER (version 9.25) - SWISS-MODEL (version 3.0.0)