

Summary of integrative structure determination of A structural model of the endogenous human SWI/SNF (BAF) complex bound to the nucleosome informs disease mechanisms (PDB ID: 9A0K, PDB-Dev ID: PDBDEV_00000056)

1. Model Composition	
<u>Entry composition</u>	<ul style="list-style-type: none"> - SMARCC2: Chain 2 (1214 residues) - SMARCD1: Chain D (515 residues) - ACTB: Chain B (375 residues) - H3: Chain x (136 residues) - H3: Chain X (136 residues) - ARID1A: Chain A (2285 residues) - SMARCC1: Chain 1 (1105 residues) - H4: Chain y (103 residues) - H4: Chain Y (103 residues) - H2A: Chain V (130 residues) - 601 dna fwd: Chain p (196 residues) - SMARCE1: Chain E (411 residues) - H2A: Chain v (130 residues) - H2B: Chain W (126 residues) - H2B: Chain w (126 residues) - SMARCA4: Chain 4 (1647 residues) - 601 dna rev: Chain q (196 residues) - DPF2: Chain P (391 residues) - ACTL6A: Chain 6 (429 residues) - SMARCB1: Chain b (385 residues)
	<ul style="list-style-type: none"> - 3DEM volume, File: 10.5281/zenodo.3998811 - Crosslinking-MS data, Linker name and number of cross-links: BS3, 1261 cross-links - 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 - 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 - 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 - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available

[Datasets used for modeling](#)

- Comparative model, template PDB ID: Not available
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- Comparative model, template PDB ID: Not available
- De Novo model, File: 10.5281/zenodo.3998811
- De Novo model, File: 10.5281/zenodo.3998811
- Experimental model, PDB ID: 6UXV
- Experimental model, PDB ID: 6UXV
- Experimental model, PDB ID: 6UCH
- Experimental model, PDB ID: 6UXV
- Experimental model, PDB ID: 5X0Y
- Experimental model, PDB ID: 5X0Y
- Experimental model, PDB ID: 5X0Y
- Experimental model, PDB ID: 6UXV
- Experimental model, PDB ID: 5X0Y
- Experimental model, PDB ID: 5X0Y
- Experimental model, PDB ID: 6UXV
- Experimental model, PDB ID: 4I6M
- Experimental model, PDB ID: 5X0Y
- Experimental model, PDB ID: 6UXV
- Experimental model, PDB ID: 4I6M
- Experimental model, PDB ID: 5X0Y
- Experimental model, PDB ID: 5X0Y
- Experimental model, PDB ID: 6UXV
- Experimental model, PDB ID: 5X0Y
- Experimental model, PDB ID: 5X0Y
- Experimental model, PDB ID: 4I6M
- Experimental model, PDB ID: 5X0Y
- 3DEM volume, EMDB: EMD-22476
- 3DEM volume, EMDB: EMD-22478

2. Representation	
Resolution	Atomic
Number of rigid bodies , flexible units	23, 0
<i>Rigid bodies</i>	<ul style="list-style-type: none"> - B: 1-375 - 6: 1-429 - A: 1-2285 - P: 1-88 - 4: 1-16471-16471-1647 - b: 1-3851-385 - 1: 1-1105 - 2: 1-1214 - D: 1-515 - E: 220-298 - V: 1-130 - W: 1-126 - X: 1-136 - Y: 1-103 - v: 1-130 - w: 1-126 - x: 1-136 - y: 1-103 - p: 1-196 - q: 1-196

Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: BS3, 1261 cross-links - 1 unique EM3DRestraint: None
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 27, Number of sidechain outliers = 10
Model quality: assessment of excluded volume	Not applicable
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	Production sampling
Name	Monte Carlo
2. Method	trRosetta
Name	trRosetta
3. Method	Rosetta Hybridize
Name	Rosetta Hybridize
Software	- Rosetta (version Rosetta version unknown:ff8ee24ee5f65423d5064cba818ede41d012fa8; 2020-08-10 10:39:53 -0700 from git@github.com:RosettaCommons/main.git) - trRosetta (version 1.0.0) - HHPred (version website)