

Summary of integrative structure determination of CLOCK-BMAL1 bound to a nucleosome at SHL -6.2 (PDB ID: 9A3O, PDB-Dev ID: PDBDEV_00000209)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Histone H3.1: chain(s) A, E (139 residues) - Histone H4: chain(s) B, F (106 residues) - Histone H2A: chain(s) C, G (133 residues) - Histone H2B: chain(s) D, H (128 residues) - DNA (128-MER): chain(s) I (153 residues) - DNA (128-MER): chain(s) J (153 residues) - Circadian locomotor output cycles protein kaput: chain(s) K [M] (375 residues) - Basic helix-loop-helix ARNT-like protein 1: chain(s) L [N] (384 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, PRIDE: PXD033181 - 3DEM volume, EMDB: EMD-17155 - Experimental model, PDB: 6T93 - Experimental model, PDB: 4F3L - Experimental model, PDB: 8OSJ
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 16
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSSO, 42 crosslinks - 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)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 0.92 - Ramachandran outliers: 22 - Sidechain outliers: 10
Fit to data used for modeling	Satisfaction of crosslinks: 0.00%

<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>	Manual fitting
2. <i>Name</i>	Rosetta Dock with crosslink filter and density scoring
<i>Software</i>	<ul style="list-style-type: none"> - Coot (version 0.9.6) - Rosetta (version Not available)