

Summary of integrative structure determination of CLOCK-BMAL1 bound to the native Por nucleosome (PDB ID: 9A3P, PDB-Dev ID: PDBDEV_00000210)

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 (147-MER): chain(s) I (147 residues) - DNA (147-MER): chain(s) J (147 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-17160 - Experimental model, PDB: 6T93 - Experimental model, PDB: 4F3L - Experimental model, PDB: 8OSL
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 22
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSSO, 59 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: 2.34 - Ramachandran outliers: 43 - Sidechain outliers: 29
Fit to data used for modeling	Satisfaction of crosslinks: 0.00%

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. Name	MDFF with distance and map restraints
Software	<ul style="list-style-type: none">- ChimeraX/Isolde (version Not available)- Coot (version 0.9.6)