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	- DNA (128-MER): Chain J (153 residues) - Histone H2A: Chain G (133 residues) - Histone H4: Chain F (106 residues) - Histone H3.1: Chain E (139 residues) - Circadian locomoter output cycles protein kaput: Chain K (84 residues) - Basic helix-loop-helix ARNT-like protein 1: Chain L (8 residues) - Histone H3.1: Chain A (139 residues) - Circadian locomoter output cycles protein kaput: Chain K (11 residues) - Basic helix-loop-helix ARNT-like protein 1: Chain L (71 residues) - Histone H2B: Chain D (128 residues) - Histone H2A: Chain C (133 residues) - Histone H2B: Chain H (128 residues) - DNA (128-MER): Chain I (153 residues) - Histone H4: Chain B (106 residues) - Basic helix-loop-helix ARNT-like protein 1: Chain L (305 residues) - Circadian locomoter output cycles protein kaput: Chain K (280 residues)
Datasets used for modeling	- Crosslinking-MS data, Linker name and number of cross-links: DSSO, 42 cross-links - 3DEM volume, EMDB: EMD-17155 - Experimental model, PDB ID: 6T93 - Experimental model, PDB ID: 4F3L - Experimental model, PDB ID: 8OSJ
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 16
Flexible units	- A: 1-139 - E: 1-139 - B: 1-106 - F: 1-106 - C: 1-133 - G: 1-133 - D: 1-128 - H: 1-128 - I: 1-153 - J: 1-153 - K: 1-84, 85-364, 365-375 - L: 1-71, 72-376, 377-384
Structural coverage (rigid bodies)	100%
3. Restraints	

Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSSO, 42 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 = 0.92, Number of Ramachandran outliers = 22, Number of sidechain outliers = 15
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	Manual fitting
Name	Manual fitting
2. Method	Rosetta Dock with crosslink filter and density scoring
Name	Rosetta Dock
Software	- Coot (version 0.9.6) - Rosetta (version Not available)