Table 1: Summary of Integrative Structure Determination of Histones H3-H4 dimer

1) Gathering information	
Prior models	h3 comparative model, template 1TZY:G h4 comparative model, template 1TZY:H
Physical principles and statistical preferences	Excluded volume Sequence connectivity
Experimental data	170 pE-MAP derived distance restraints
2) Representing the system	
Composition (number of copies)	h3: 1 h4: 1
Atomic (structured) components	h3: 39-136 h4: 20-103
Unstructured components	None
Resolution of structured components	1 [R1] residue per bead
Resolution of unstructured components	None
Structural coverage	100.0 %
Rigid body (RB) definitions	RB1: $h3_{39-136}$ RB2: $h4_{20-103}$
Spatial restraints encoded into scoring function	Excluded volume; applied to the R1 representation Sequence connectivity; applied to the R1 representation pE-MAP MIC pair-restraints; applied to the R1 representation
3) Structural Sampling	
Sampling method	Replica Exchange Gibbs sampling, based on Metropolis Monte Carlo
Replica exchange temperature range	1.0 - 2.5
Number of replicas	4
Number of runs	60
Number of structures generated	2500000
Movers for rigid bodies	Random translation up to 0.3 Å Random rotation up to 0.1 radians
Movers for flexible string of bead	Random translation up to 4.0 Å
CPU time	4 hours on 20 processors
4) Validating the model	
Models selected for validation	
Number of models after equilibration	2500000
Number of models that satisfy the input information	1162507
Number of structures in samples A/B	639091/523416
p-value of non-parametric Kolmogorov-Smirnov two-sample test	0.006 (threshold p-value > 0.05)
Kolmogorov-Smirnov two-sample test statistic, D	0.96
Thoroughness of the structural sampling	
Sampling precision	2.03 Å
Homogeneity of proportions χ^2 test (p-value)/Cramers V value	0.679/0.006 (thresholds: p-value>0.05 OR Cramer's V<0.1)
Number of clusters	1
Cluster populations	cluster 1 : 98.6 %
Cluster precisions	cluster 1 : 1.04 Å
Average cross-correlation between localization probability densities of samples A and B	cluster 1: 1.0
Validation by information used for modeling	
Percent of sequence connectivity restraints satisfied per structure	99 %
Percent pE-MAP restraints satisfied per structure	87 %
Percent of excluded volume restraints satisfied per structure	99 %
5) Benchmark	
Structural accuracy (95 % CI)	3.8 (2.6-5.1) Å
PDB used for benchmark	1ID3
6) Software and data availability	
Software	
Modeling programs	IMP PMI module, version develop-39c22a602

	Integrative Modeling Platform (IMP), version develop-39c22a602
	MODELLER, version 9.21
Modeling scripts	https://github.com/salilab/pemap
Homology detection and structure prediction	HHPred, version 2.0.16
Visualization and plotting	UCSF Chimera, version 1.10
	Matplotlib, version 3.0.3
Data	
PDB-dev accesion code	TBD
pE-MAP data deposition	https://github.com/salilab/pemap