Table 2: Summary of Integrative Structure Determination of RNAPII rpb1-rpb2 dimer

1) Gathering information	
Prior models	rpb1 comparative model, template 6GMH:A rpb2 comparative model, template 4AYB:B
Physical principles and statistical preferences	Excluded volume Sequence connectivity
Experimental data	123 pE-MAP derived distance restraints
2) Representing the system	
Composition (number of copies)	rpb1: 1 rpb2: 1
Atomic (structured) components	rpb1: 13-58, 82-105, 120-143, 173-184, 200-551, 565-589, 606-1077, 1098-1105, 1119-1171, 1191-1240, 1256-1286, 1304-1404 rpb2: 24-68, 88-139, 162-301, 314-565, 579-639, 655-661, 681-709, 740-871, 887-917, 934-1099
Unstructured components	rpb1: 1-12, 59-81, 106-119, 144-172, 185-199, 552-564, 590-605, 1078-1097, 1106-1112, 1113-1118, 1172-1190, 1241-1255, 1287-1303 rpb2: 1-23, 69-87, 140-161, 302-313, 566-578, 640-654, 662-680, 710-739, 872-886, 918-933
Resolution of structured components	1 [R1] residue per bead
Resolution of unstructured components	10 [R10] residues per bead
Structural coverage	85.07 %
Rigid body (RB) definitions	RB1: $rpb1_{1-1105}$ RB2: $rpb1_{1113-1404}$ RB3: $rpb2_{1-1099}$
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	8
Number of runs	60
Number of structures generated	3600000
Movers for rigid bodies	Random translation up to 2.0 Å Random rotation up to 0.2 radians
Movers for flexible string of bead	Random translation up to 4.0 Å
CPU time	36 hours on 20 processors
4) Validating the model	
Models selected for validation	
Number of models after equilibration	3600000
Number of models that satisfy the input information	425380
Number of structures in samples A/B	210367/215013
p-value of non-parametric Kolmogorov-Smirnov two-sample test	0.012 (threshold p-value > 0.05)
Kolmogorov-Smirnov two-sample test statistic, D	0.23
Thoroughness of the structural sampling	
Sampling precision	14.84 Å
Homogeneity of proportions χ^2 test (p-value)/Cramers V value	0.000/0.099 (thresholds: p-value>0.05 OR Cramer's V<0.1)
Number of clusters	2
Cluster populations	cluster 1 : 81.7 % cluster 2 : 14.8 %
Cluster precisions	cluster 1 : 9.78 Å cluster 2 : 9.92 Å
Average cross-correlation between localization probability densities of samples A and B	cluster 1: 0.76 cluster 2: 0.84
Validation by information used for modeling	
Percent of sequence connectivity restraints satisfied per structure	99 %
Percent pE-MAP restraints satisfied per structure	95 %

Percent of excluded volume restraints satisfied per structure	99 %
5) Benchmark	
Structural accuracy (95 % CI)	16.8 (12.5-23.2) Å
PDB used for benchmark	1I3Q
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