Table 3: Summary of Integrative Structure Determination of Bacterial RNAP subunits rpob and rpoc

1) Gathering information	
Prior models	X-ray structure 4YG2
Physical principles and statistical preferences	Excluded volume Sequence connectivity
Experimental data	63 conditional genetics derived distance restraints
2) Representing the system	
Composition (number of copies)	rpob: 1 rpoc: 1
Atomic (structured) components	rpob: 3-1342 rpoc: 8-931, 1135-1374
Unstructured components	rpob: 1-2 rpoc: 932-1134
Resolution of structured components	1 [R1] residue per bead
Resolution of unstructured components	20 [R20] residues per bead
Structural coverage	92.49 %
Rigid body (RB) definitions	RB1: rpob_{3-1342} RB2: rpoc_{8-931},$\text{rpoc}_{1135-1374}$
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	50
Number of structures generated	2500000
Movers for rigid bodies	Random translation up to 1.0 Å Random rotation up to 0.2 radians
Movers for flexible string of bead	Random translation up to 4.0 Å
CPU time	16 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	382928
Number of structures in samples A/B	189328/193600
p-value of non-parametric Kolmogorov-Smirnov two-sample test	0.035 (threshold p-value > 0.05)
Kolmogorov-Smirnov two-sample test statistic, D	0.0
Thoroughness of the structural sampling	
Sampling precision	23.03 Å
Homogeneity of proportions χ^2 test (p-value)/Cramers V value	1.0/0.0 (thresholds: p-value>0.05 OR Cramer's V<0.1)
Number of clusters	1
Cluster populations	cluster 1 : 91.5 %
Cluster precisions	cluster 1 : 5.25 Å
Average cross-correlation between localization probability densities of samples A and B	cluster 1: 0.71
Validation by information used for modeling	
Percent of sequence connectivity restraints satisfied per structure	99 %
Percent pE-MAP restraints satisfied per structure	92 %
Percent of excluded volume restraints satisfied per structure	99 %
5) Benchmark	
Structural accuracy (95 % CI)	14.3 (12.2-18.4) Å
PDB used for benchmark	4YG2
6) Software and data availability	
Software	
Modeling programs	IMP PMI module, version develop-39c22a602

	Integrative Modeling Platform (IMP), version develop-39c22a602
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