

Table 1: Summary of Integrative Structure Determination of Bacterial RNAP subunits rpob and rpoc

<b>1) Gathering information</b>	
<i>Prior models</i>	X-ray structure 4YG2
<i>Physical principles and statistical preferences</i>	Excluded volume Sequence connectivity
<i>Experimental data</i>	63 conditional genetics derived distance restraints
<b>2) Representing the system</b>	
<i>Composition (number of copies)</i>	rpob: 1 rpoc: 1
<i>Atomic (structured) components</i>	rpob: 3-1342 rpoc: 8-931, 1135-1374
<i>Unstructured components</i>	rpob: 1-2 rpoc: 932-1134
<i>Resolution of structured components</i>	1 [R1] residue per bead
<i>Resolution of unstructured components</i>	20 [R20] residues per bead
<i>Structural coverage</i>	92.49 %
<i>Rigid body (RB) definitions</i>	RB1: rpob <sub>3-1342</sub> RB2: rpoc <sub>8-931</sub> , rpoc <sub>1135-1374</sub>
<i>Spatial restraints encoded into scoring function</i>	Excluded volume; applied to the R1 representation Sequence connectivity; applied to the R1 representation pE-MAP MIC pair-restraints; applied to the R1 representation
<b>3) Structural Sampling</b>	
<i>Sampling method</i>	Replica Exchange Gibbs sampling, based on Metropolis Monte Carlo
<i>Replica exchange temperature range</i>	1.0 - 2.5
<i>Number of replicas</i>	8
<i>Number of runs</i>	50
<i>Number of structures generated</i>	2500000
<i>Movers for rigid bodies</i>	Random translation up to 1.0 Å Random rotation up to 0.2 radians
<i>Movers for flexible string of bead</i>	Random translation up to 4.0 Å
<i>CPU time</i>	16 hours on 20 processors
<b>4) Validating the model</b>	
<b>Models selected for validation</b>	
<i>Number of models after equilibration</i>	2500000
<i>Number of models that satisfy the input information</i>	382928
<i>Number of structures in samples A/B</i>	189328/193600
<i>p-value of non-parametric Kolmogorov-Smirnov two-sample test</i>	0.035 (threshold p-value > 0.05)
<i>Kolmogorov-Smirnov two-sample test statistic, D</i>	0.0
<b>Thoroughness of the structural sampling</b>	
<i>Sampling precision</i>	23.03 Å
<i>Homogeneity of proportions <math>\chi^2</math> test (p-value)/Cramers V value</i>	1.0/0.0 (thresholds: p-value>0.05 OR Cramer's V<0.1)
<i>Number of clusters</i>	1
<i>Cluster populations</i>	cluster 1 : 91.5 %
<i>Cluster precisions</i>	cluster 1 : 5.25 Å
<i>Average cross-correlation between localization probability densities of samples A and B</i>	cluster 1: 0.71
<b>Validation by information used for modeling</b>	
<i>Percent of sequence connectivity restraints satisfied per structure</i>	99 %
<i>Percent pE-MAP restraints satisfied per structure</i>	92 %
<i>Percent of excluded volume restraints satisfied per structure</i>	99 %
<b>5) Benchmark</b>	
<i>Structural accuracy (95 % CI)</i>	14.3 (12.2-18.4) Å
<b>6) Software and data availability</b>	
<b>Software</b>	
<i>Modeling programs</i>	IMP PMI module, version develop-39c22a602 Integrative Modeling Platform (IMP), version develop-39c22a602

<i>Modeling scripts</i>	<a href="https://github.com/salilab/pemap">https://github.com/salilab/pemap</a>
<i>Homology detection and structure prediction</i>	HHPred, version 2.0.16
<i>Visualization and plotting</i>	UCSF Chimera, version 1.10
	Matplotlib, version 3.0.3
<b>Data</b>	
<i>PDB-dev accession code</i>	TBD
<i>pE-MAP data deposition</i>	<a href="https://github.com/salilab/pemap">https://github.com/salilab/pemap</a>