

Table 9: Summary of Integrative Structure Determination of Bacterial RNAP subunits Rpob and Rpoc

1) Gathering information	
<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
2) Representing the system	
<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 ₃₋₁₃₄₂ RB2: rpoc ₈₋₉₃₁ , rpoc ₁₁₃₅₋₁₃₇₄
<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
3) Structural Sampling	
<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>	4
<i>Number of runs</i>	50
<i>Number of structures generated</i>	2500000
<i>Movers for flexible string of bead</i>	Random translation up to 4.0 Å
<i>CPU time</i>	16 hours on 20 processors
4) Validating the model	
Models selected for validation	
<i>Number of models after equilibration</i>	2500000
<i>Number of models that satisfy the input information</i>	656275
<i>Number of structures in samples A/B</i>	407275/249000
<i>p-value of non-parametric Kolmogorov-Smirnov two-sample test</i>	0.251 (threshold p-value > 0.05)
<i>Kolmogorov-Smirnov two-sample test statistic, D</i>	0.0
Thoroughness of the structural sampling	
<i>Sampling precision</i>	9.38 Å
<i>Homogeneity of proportions χ^2 test (p-value)/Cramers V value</i>	1.000/0.000 (thresholds: p-value>0.05 OR Cramer's V<0.1)
<i>Number of clusters</i>	1
<i>Cluster populations</i>	cluster 1 : 100.0 %
<i>Cluster precisions</i>	cluster 1 : 6.61 Å
<i>Average cross-correlation between localization probability densities of samples A and B</i>	cluster 1: 0.68
Validation by information used for modeling	
<i>Percent of sequence connectivity restraints satisfied per structure</i>	99 %
<i>Percent pE-MAP restraints satisfied per structure</i>	94 %
<i>Percent of excluded volume restraints satisfied per structure</i>	99 %
5) Benchmark	
<i>Structural accuracy (95 % CI)</i>	15.0 (12.1-18.2) Å
<i>PDB used for benchmark</i>	4YG2
6) Software and data availability	
<i>Modeling programs</i>	IMP PMI module, version develop-39c22a602 Integrative Modeling Platform (IMP), version develop-39c22a602
<i>Modeling scripts and data</i>	https://integrativemodeling.org/systems/pemap
<i>Homology detection and structure prediction</i>	HHPred, version 2.0.16

