

Table 9: Summary of the Pks13 dimer integrative structure modeling

<b>1) Gathering information</b>	
<i>Prior models</i>	2-fold symmetry derived from cryo-EM structure
<i>Physical principles and statistical preferences</i>	Excluded volume Sequence connectivity
<i>Experimental data</i>	57 DSS0 Atomic structure from cryo-EM map; PDB TBD
<b>2) Representing the system</b>	
<i>Atomic (structured) components</i>	Pks13: 1-76, 89-228, 229-232, 233-529, 588-835, 836-838, 839-1074, 1078-1173, 1238-1356, 1461-1535, 1539-1816, 1-76, 89-228, 229-232, 233-529, 588-835, 836-838, 839-1074, 1078-1173, 1238-1356, 1461-1535, 1539-1816
<i>Unstructured components</i>	Pks13: 77-88, 530-587, 1075-1077, 1174-1237, 1357-1460, 1536-1538, 77-88, 530-587, 1075-1077, 1174-1237, 1357-1460, 1536-1538
<i>Resolution of structured components</i>	1 [R1] residue per bead
<i>Resolution of unstructured components</i>	10 [R10] residues per bead
<i>Structural coverage</i>	86.77 %
<i>Rigid body (RB) definitions</i>	RB1: Pks13 <sub>1-76</sub> RB2: Pks13 <sub>89-228</sub> , Pks13 <sub>229-232</sub> , Pks13 <sub>233-529</sub> , Pks13 <sub>588-835</sub> , Pks13 <sub>836-838</sub> RB3: Pks13 <sub>1078-1173</sub> RB4: Pks13 <sub>1238-1356</sub> RB5: Pks13 <sub>1461-1535</sub> RB6: Pks13 <sub>1539-1816</sub> RB7: Pks13 <sub>1-76</sub> RB8: Pks13 <sub>89-228</sub> , Pks13 <sub>229-232</sub> , Pks13 <sub>233-529</sub> , Pks13 <sub>588-835</sub> , Pks13 <sub>836-838</sub> RB9: Pks13 <sub>1078-1173</sub> RB10: Pks13 <sub>1238-1356</sub> RB11: Pks13 <sub>1461-1535</sub> RB12: Pks13 <sub>1539-1816</sub>
<i>Resolution of disordered regions</i>	10 [R10] residues per bead
<i>Composition (number of copies of Pks13)</i>	2
<i>Spatial restraints encoded into scoring function</i>	Excluded volume; applied to the R1 representation Sequence connectivity; applied to the R1 representation Cross-link restraints; applied to the R1 representation
<b>3.1) Enumeration of threading of degrees of freedom</b>	
<b>3.2) 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>	100
<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>	22 hours on 80 processors
<b>4.1) Validating the threading models</b>	
<b>4.2) Validating the Pom152 ring models</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>	229554
<i>Number of structures in samples A/B</i>	112886/116668
<i>p-value of non-parametric Kolmogorov-Smirnov two-sample test</i>	0.02 (threshold p-value > 0.05)
<i>Kolmogorov-Smirnov two-sample test statistic, D</i>	1.0
<b>Thoroughness of the structural sampling</b>	
<i>Sampling precision</i>	61.37 Å
<i>Homogeneity of proportions <math>\chi^2</math> test (p-value)/Cramers V value</i>	0.000/0.067 (thresholds: p-value>0.05 OR Cramer's V<0.1)
<i>Number of clusters</i>	3
<i>Cluster precisions</i>	cluster 1 : 55.0 % cluster 2 : 21.7 %

<i>Average cross-correlation between localization probability densities of samples A and B</i>	cluster 3 : 19.1 % cluster 1: 0.89
<i>Cluster populations</i>	cluster 2: 0.72 cluster 3: 0.7 cluster 1 : 52.7 % cluster 2 : 21.7 % cluster 3 : 20.9 %
<b>Validation by information used for modeling</b>	
<i>Percent of sequence connectivity restraints satisfied per structure</i>	99 %
<i>Percent cross-link restraints satisfied by ensemble</i>	91 %
<i>Percent of excluded volume restraints satisfied per structure</i>	99 %
<b>6) Software and data availability</b>	
<b>Software</b>	
<i>Modeling programs</i>	IMP PMI module, version 2.16.0 Integrative Modeling Platform (IMP), version 2.16.0 <a href="https://github.com/integrativemodeling/Pks13">https://github.com/integrativemodeling/Pks13</a>
<i>Modeling scripts</i>	AlphaFold2
<i>Structure prediction</i>	UCSF Chimera
<i>Visualization and plotting</i>	Matplotlib, version 3.0.3
<b>Data</b>	
<i>PDB-dev accession code</i>	TBD