nature portfolio

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Reporting Summary

Nature Portfolio wishes to improve the reproducibility of the work that we publish. This form provides structure for consistency and transparency in reporting. For further information on Nature Portfolio policies, see our <u>Editorial Policies</u> and the <u>Editorial Policy Checklist</u>.

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FOI :	ali St	atistical analyses, commit that the following items are present in the rigure regend, table regend, main text, or Methods section.
n/a	Cor	nfirmed
\boxtimes		The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement
X		A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly
	\boxtimes	The statistical test(s) used AND whether they are one- or two-sided Only common tests should be described solely by name; describe more complex techniques in the Methods section.
X		A description of all covariates tested
	\boxtimes	A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons
\boxtimes		A full description of the statistical parameters including central tendency (e.g. means) or other basic estimates (e.g. regression coefficient) AND variation (e.g. standard deviation) or associated estimates of uncertainty (e.g. confidence intervals)
\boxtimes		For null hypothesis testing, the test statistic (e.g. <i>F</i> , <i>t</i> , <i>r</i>) with confidence intervals, effect sizes, degrees of freedom and <i>P</i> value noted <i>Give P values as exact values whenever suitable.</i>
\boxtimes		For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings
\boxtimes		For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes
\boxtimes		Estimates of effect sizes (e.g. Cohen's d, Pearson's r), indicating how they were calculated
		Our web collection on <u>statistics for biologists</u> contains articles on many of the points above.

Software and code

Policy information about availability of computer code

Data collection

SerialEM

Data analysis

CryoSPARC v2.12, Relion v3.0, Chimera v1.15, Chimera X - Isolde v1.4, Phenix v1.20.1-4489, Coot v0.9.6, MOLE v2, Analyst vTF1.5, MSConvert (ProteoWizard), ProteinProspector v 5.19.1, XLTools, xiNET, Integrative Modeling Platform

For manuscripts utilizing custom algorithms or software that are central to the research but not yet described in published literature, software must be made available to editors and reviewers. We strongly encourage code deposition in a community repository (e.g. GitHub). See the Nature Portfolio guidelines for submitting code & software for further information.

Data

Policy information about availability of data

All manuscripts must include a data availability statement. This statement should provide the following information, where applicable:

- Accession codes, unique identifiers, or web links for publicly available datasets
- A description of any restrictions on data availability
- For clinical datasets or third party data, please ensure that the statement adheres to our policy

all data obtained in this study have been deposited as noted in the manuscript. all data obtained in this study have been deposited as noted in the manuscript. The atomic coordinates for six structures of pks13 have been deposited in the Protein Data Bank with the accession codes 7UK4, 8CUY, 8CV1, 8CUZ, 8CV0. The corresponding maps have been deposited in the Electron Microscopy Data Bank with the accession codes EMD-26574, EMD-27002, EMD27005, EMD-27003,

		rative modeling are freely available at https://github.com/integrativemodeling/Pks13. The details about the approach are given		
Human rese	arch part	ticipants		
Policy information	about <u>studies</u>	s involving human research participants and Sex and Gender in Research.		
Reporting on sex and gender Not Applicable		Not Applicable		
		Not Applicable		
		ot Applicable		
Ethics oversight		Not Applicable		
_	ation on the app	proval of the study protocol must also be provided in the manuscript.		
Please select the o	ne below that	eporting t is the best fit for your research. If you are not sure, read the appropriate sections before making your selection. Behavioural & social sciences		
		cudy design se points even when the disclosure is negative.		
Sample size	Several million are reported.	ons of particle images were combined into the CryoEM analysis. They were classified into the different states whose structures I.		
Data exclusions	do not fit th e were from po since they we	woEM analysis, many thousands of images are classified according to their quality. Those images that do not have suitable quality, or it the classes are excluded from further averaging. As to the chemical cross linking, we excluded large molecular weight species that om potential aggregates of multiple molecules, cross linked residues that are too far apart for within a dimeric Pks13 were excluded ey were presumed to arise from multimeric assemblies of PKS molecules and not relevant to intramolecular dynamics. (detailed in s, and Fig S9, S10, and Extended Fig 10.		
Replication		eplication was that the crosslinking experiment was done twice but at two different temperatures, giving non-equivalent data that compared statistically. see Supp Fig 9. caption		
Randomization		1,400,000 Images of Single particles for the di-domain structures (KS-AT) and 1,200,000 for each of the other 5 structures, were classified according to standard procedures in cryoEM imaging by classification into separate classes that are gleaned from 100% of the particle image ets.		
Blinding	There was no	blinding. images of particles were picked according to classification into classes as is the standard in cryoEM imaging		
We require informati	on from author ted is relevant t perimental	specific materials, systems and methods rs about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, to your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response. Systems Methods n/a Involved in the study		
Antibodies		ChIP-seq		
Eukaryotic cell lines		Flow cytometry		
Palaeontol	logy and archae	eology MRI-based neuroimaging		

Animals and other organisms

Dual use research of concern

Clinical data