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Reporting Summary

Nature Research 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 Research policies, see <u>Authors & Referees</u> and the <u>Editorial Policy Checklist</u>.

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1016	an statistical analyses, commit that the following items are present in the figure regend, table regend, main text, or interious section.
n/a	Confirmed
	\mathbf{x} The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement
	A statement on whether measurements were taken from distinct samples or whether the same sample was measured repeatedly
×	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.
×	A description of all covariates tested
	🗴 A description of any assumptions or corrections, such as tests of normality and adjustment for multiple comparisons
	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)
×	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>
x	For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings
×	For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes
×	Estimates of effect sizes (e.g. Cohen's <i>d</i> , Pearson's <i>r</i>), 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 LS-CAT Synchrotron, MassHunter

Data analysis HKL-2000, Phenix, Coot, SBGrid, Pymol, Graphpad v5.0a, Excel v16.36, Cytoscape v3.7.1

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/reviewers. We strongly encourage code deposition in a community repository (e.g. GitHub). See the Nature Research 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 list of figures that have associated raw data
- A description of any restrictions on data availability

Protein coordinates and structure factors have been submitted to the Protein Data Bank under accession codes 6WN3 (SxtT) [http://www.rcsb.org/structure/6WN3], 6WNC (GxtA) [http://www.rcsb.org/structure/6WNC], 6WNB (ddSTX-bound SxtT) [http://www.rcsb.org/structure/6WNB], and 6WND (ddSTX-bound GxtA) [http://www.rcsb.org/structure/6WND]. The source data underlying Supplementary Figs 10, 11, and 12 are provided as a Source Data file. Other data are available in the Supplementary Information and from the corresponding authors upon reasonable request.

Field-specific reporting

Life sciences study design

All studies must disclose on these points even when the disclosure is negative.					
Sample size	All reactions were conducted in triplicate for satisfactory technical reproducibility.				
Data exclusions	No data was excluded.				
Replication	All experiments were conducted in triplicate where each replicate was successful.				
Randomization	Randomization was not necessary due to the nature of the study.				
Blinding	Blinding was not necessary due to the nature of the study.				

Reporting for specific materials, systems and methods

We require information from authors about some types of materials, experimental systems and methods used in many studies. Here, indicate whether each material, system or method listed is relevant to your study. If you are not sure if a list item applies to your research, read the appropriate section before selecting a response.

n/a Involved in the study n/a Involved in the study	
X Antibodies X ChIP-seq	
Eukaryotic cell lines	
Palaeontology MRI-based neuroimaging	
Animals and other organisms	
Human research participants	
Clinical data	