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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 our Editorial Policies and the Editorial Policy Checklist.

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| For | all statistical and | alyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section. | | | |
|--|--|---|--|--|--|
| n/a | Confirmed | | | | |
| \boxtimes | \Box The exact sample size (n) for each experimental group/condition, given as a discrete number and unit of measurement | | | | |
| \boxtimes | A stateme | nt 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. | | | | |
| \boxtimes | A descripti | ion 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 Give <i>P</i> values as exact values whenever suitable. | | | | |
| \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 <u>availability of computer code</u> | | | | | |
| Data collection SFX data was collected during the LCLS beamtime at SLAC National Accelerator Laboratory through PS | | SFX data was collected during the LCLS beamtime at SLAC National Accelerator Laboratory through PSOCAKE for determining the initial | | | |

SFX data was collected during the LCLS beamtime at SLAC National Accelerator Laboratory through PSOCAKE for determining the initial diffraction geometry of the detector. Synchrotron X-ray diffraction data were collected with a Pilatus 6M detector at the Stanford Synchrotron Radiation Lightsource.

Data analysis

All SFX diffraction patterns were selected using CHEETAH software; indexed by using the CrystFEL software; used as indexing algorithms via XGANDALF, DIRAX, MOSFLM and XDS softwares; integrated and merged using PARTIALATOR; scaled and cut using the TRUNCATE program from the CCP4 suite. All cryo-synchrotron structure, X-ray diffraction data were processed with XDS package for indexing and scaled by using XSCALE.

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 Research guidelines for submitting code & software for further information.

Data

Policy information about <u>availability of data</u>

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

https://doi.org/10.2210/pdb7EK8/pdb; https://doi.org/10.2210/pdb7EK9/pdb

| Field-specific reporting | | | | | | |
|---|--|--|--|--|--|--|
| Please select the one below that is the best fit for your research. If you are not sure, read the appropriate sections before making your selection. | | | | | | |
| Life sciences | Behavioural & social | sciences Ecological, evolutionary & environmental sciences | | | | |
| For a reference copy of t | he document with all sections, see <u>nature.c</u> | om/documents/nr-reporting-summary-flat.pdf | | | | |
| | | | | | | |
| Life sciences study design | | | | | | |
| All studies must disclose on these points even when the disclosure is negative. | | | | | | |
| Sample size | Protein samples were purchased with | nout a specific sample size and crystallized by sitting-drop microbatch screening under oil. | | | | |
| Data exclusions | The complete reflection intensity was | s cut using the TRUNCATE program from the CCP4 suite for SFX structure. | | | | |
| Replication | Replication was provided using 72 we | ell Terasaki crystallization plates. | | | | |
| Randomization | N/A | | | | | |
| Blinding | N/A | | | | | |
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| 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. | | | | | | |
| Materials & experimental systems | | Methods | | | | |
| n/a Involved in the study | | n/a Involved in the study | | | | |
| Antibodies | | ChIP-seq | | | | |
| Eukaryotic cell lines | | Flow cytometry | | | | |
| Palaeontology and archaeology | | MRI-based neuroimaging | | | | |
| Animals an | Animals and other organisms | | | | | |

Human research participants

Clinical data
Dual use research of concern