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 Editorial Policies and the Editorial Policy Checklist.

Statistics

For all statistical analyses, confirm that the following items are present in the figure legend, table legend, main text, or Methods section.

n/a	Confirmed	
☐	☒	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. *F*, *t*, *r*) with confidence intervals, effect sizes, degrees of freedom and *P* value noted *Give P values as exact values whenever suitable.*
☒	☐	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 *d*, Pearson's *r*), indicating how they were calculated

Our web collection on statistics for biologists contains articles on many of the points above.

Software and code

Policy information about availability of computer code

Data collection	TopSpin 3.2
Data analysis	pynmrstar 3.3.1 HYDRONMR 7c PINT v1.0 ChemEx (https://github.com/gbouvignies/chemex) ESMFold; ESM-2 (https://github.com/facebookresearch/ESM) AlphaFold2 via ColabDesign (https://github.com/sokrypton/ColabDesign.git@gamma) ProDy v 2.0 PlotDigitizer (https://plotdigitizer.com/) Dyna-1 code: https://github.com/WaymentSteeleLab/Dyna-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 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

The mBMRB training set, RelaxDB, and RelaxDB-CPMG datasets are publicly available for noncommercial use at https://github.com/WaymentSteeleLab/Dyna-1 and at https://huggingface.co/spaces/gelnesr/Dyna-1, doi: 10.57967/hf/9277. Raw data for CPMG relaxation dispersion for the two prospective proteins characterized in this study are deposited at 10.5281/zenodo.20834076.
NMR chemical shift assignments used to construct the mBMRB dataset were obtained from the Biological Magnetic Resonance Data Bank (BMRB; https://bmrb.io). Protein structures used in this study were obtained from the RCSB Protein Data Bank (PDB; https://rcsb.org); specific entries used include PDB IDs 4AKE, 3TG3, 2LUO, 1UPA, and 1U2P. BMRB entries for the prospective test proteins are BMRB:11466 (chitinase 19) and BMRB:51320 (yjbJ).

Research involving human participants, their data, or biological material

Policy information about studies with human participants or human data. See also policy information about sex, gender (identity/presentation), and sexual orientation and race, ethnicity and racism.

Reporting on sex and gender	N/A
Reporting on race, ethnicity, or other socially relevant groupings	N/A
Population characteristics	N/A
Recruitment	N/A
Ethics oversight	N/A

Note that full information on the approval of the study protocol must also be provided in the manuscript.

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 the document with all sections, see nature.com/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	Our sample sizes for training and evaluation were based on data availability rather than statistical power calculations. We curated 133 protein datasets with standardized Rex measurements in RelaxDB, and 9,381 proteins in the mBMRB dataset. While no formal statistical methods were used to determine sample size, our rationales are as follows: the RelaxDB dataset represents the largest curated set of µs-ms dynamics from NMR relaxation data to date, and the mBMRB dataset leverages all possible missing assignment data from the BMRB, covering a broad range of proteins.
Data exclusions	Data exclusions were performed according to specific pre-established criteria. mBMRB dataset: we excluded proteins from the mBMRB dataset that used selective isotope labeling, methyl labeling, or deuteration (due to the possibility of incomplete back-exchange leading to missing peaks unrelated to dynamics). RelaxDB dataset: intrinsically disordered proteins, proteins with ligands present in experimental conditions, and proteins forming multimers under experimental conditions were excluded from RelaxDB to avoid confounding effects on Rex measurements. These exclusions were made to ensure that Rex signal reflected µs-ms motions rather than other processes.
Replication	15N CPMG relaxation dispersion experiments for the two prospective test proteins (chitinase 19 and yjbJ) were each performed once on a single purified protein sample; reproducibility within each experiment is assessed via duplicate CPMG measurements used for error estimation. NMR relaxation experiments are not conventionally replicated with independent biological replicates, sample integrity and measurement reproducibility are instead validated through internal spectral controls and fitting errors. All other analyses are computational and were performed on the RelaxDB and mBMRB datasets, which aggregate data from many independent laboratories, providing cross-laboratory reproducibility assessment.

Randomization	Randomization was not relevant to this study. The allocation of data points (i.e., proteins) into training, validation, and test sets was based on sequence identity and structural similarity thresholds to ensure independence between datasets, rather than random allocation. This approach was appropriate for the study's objectives, as it aimed to prevent data leakage and assess generalizability rather than balance covariates across experimental groups.
Blinding	Blinding was not relevant to this study. The data used (NMR datasets of missing assignments and relaxation data) are publicly available and objectively labeled based on experimental outcomes and pre-established criteria. The authors were not blinded during data processing or analysis.

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

n/a	Involved in the study
☒	☐ Antibodies
☒	☐ Eukaryotic cell lines
☒	☐ Palaeontology and archaeology
☒	☐ Animals and other organisms
☒	☐ Clinical data
☒	☐ Dual use research of concern
☒	☐ Plants

Methods

n/a	Involved in the study
☒	☐ ChIP-seq
☒	☐ Flow cytometry
☒	☐ MRI-based neuroimaging

Plants

Seed stocks	N/A
Novel plant genotypes	N/A
Authentication	N/A