

## 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](#).

### 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

Kinetics and spectroscopic analysis  
Chirscan Spectrometer Control Panel Application version 4.2.27 (Circular Dichroism)  
Spectra Manager version 2.07.02 (Build 4) (UV-Vis-based Kinetics)

X-ray crystallography  
mxCuBE 2 (X-ray data collection at P14 DESY/EMBL, Hamburg, Germany)

Mass spectrometry  
Orbitrap Exploris 480 or Q Exactive (Thermo Scientific), both coupled to a Dionex UltiMate 3000 UHPLC system (Thermo Scientific).

Analytical ultracentrifugation  
ProteomeLab XL-I, GUI 6.0 (Firmware 5.7)

Electronic structure calculations  
Gaussian16

#### Data analysis

Kinetics and spectroscopic analysis  
Pro-Data Viewer version 4.2.27 (Circular Dichroism)  
Spectra Manager version 2.07.02 (Build 4) (UV-Vis-based Kinetics)  
SigmaPlot version 11.0 (Circular Dichroism, UV-Vis-based Kinetics)

Crystallography  
XDS VERSION Mar 15, 2019 BUILT=20190315 (X-ray, data processing)  
XSCALE VERSION Jan 31, 2020 BUILT=20200417 (X-ray, data scaling)

CCP4 version 7.0.78 (X-ray, processing and refinement)  
 phenix.refine version 1.13\_2998 (structure, refinement)  
 COOT version 0.8.9.2 (structure, model building)  
 MolProbity-Server Version 4 (structure validation)  
 The PyMOL Molecular Graphics System version 1.3 (structure representation)

Electronic structure calculations  
 Gaussian16  
 Python3.1 (libraries: numpy)

Mass spectrometry data analysis  
 FreeStyle 1.3  
 MaxQuant 1.6.5.0

Analytical ultracentrifugation  
 SEDFIT version 16.2b (fitting of the raw data with the Continuous c(s) Distribution model)  
 SEDNTERP version 1.09 (calculation of extinction coefficients, partial specific volumes, density, viscosity, s 20, w correction)  
 GUSI version 1.4.6 (preparation of figures)

Phylogenetic analysis  
 MAFFT 7  
 iTOL 5  
 Jalview 2.11

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 [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

The refined structural protein models and corresponding structure-factor amplitudes are deposited under PDB accession codes 6XZ4 (NgTAL oxidized citrate 1), 6ZWJ (NgTAL oxidized citrate 2), 6ZWH (NgTAL oxidized acetate), 6ZWF (NgTAL reduced citrate), 7BOL (NgTAL oxidized low-dose), 7BBX (NgAL variant Lys8Ala) and 7BBW (NgTAL variant Cys38Ser). The structures cited in this publication (1M3Q, 3CLM, 6T3X, 5Y72) are available under their respective PDB accession codes. All other data are available on request.

## 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](https://www.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     | n.a.                                           |
| Data exclusions | n.a.                                           |
| Replication     | Measurements were repeated at least two times. |
| Randomization   | n.a.                                           |
| Blinding        | n.a.                                           |

## 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                                  |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> Antibodies                    |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> Eukaryotic cell lines         |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> Palaeontology and archaeology |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> Animals and other organisms   |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> Human research participants   |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> Clinical data                 |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> Dual use research of concern  |

Methods

|                                     |                                                 |
|-------------------------------------|-------------------------------------------------|
| n/a                                 | Involved in the study                           |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> ChIP-seq               |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> Flow cytometry         |
| <input checked="" type="checkbox"/> | <input type="checkbox"/> MRI-based neuroimaging |