## nature research

Corresponding author(s):	Kalle Gehring
Last updated by author(s):	Jun 4, 2021

## **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 <u>Editorial Policies</u> and the <u>Editorial Policy Checklist</u>.

$\overline{}$				
ς.	tα	ıΤı	ıct	ics

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
	igspace 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.
$\boxtimes$	A description of all covariates tested
$\boxtimes$	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>
$\times$	For Bayesian analysis, information on the choice of priors and Markov chain Monte Carlo settings
$\times$	For hierarchical and complex designs, identification of the appropriate level for tests and full reporting of outcomes
$\times$	$\square$ 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 MxDC (v. 2020.8.21), SoftMax Pro 5

Data analysis

MEGAX (v. 10.1.8), HKL-2000 (v. 720), PHENIX (v. 1.19.2\_4158), Coot (v. 0.9.3), PyMOL (v. 2.3.4), ORIGIN, Sedfit (v. 1501b), Sednterp, US-SOMO (v. 3167), GUSSI (v. 1.3.0), PEAKS 7, HDExaminer, Microsoft Excel (v. 16.49), Graphpad Prism (v. 9.0.2), MODELLER (v. 9.25), ProtSkin, CHARMM-GUI

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>

 $All \ manuscripts \ must \ include \ a \ \underline{data \ availability \ statement}. \ This \ statement \ should \ provide \ the \ following \ information, \ where \ applicable:$ 

- 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

Atomic coordinates and structure factors for MtCorBCBS with Mg2+-ATP, MtCorBΔC with Mg2+-ATP, and MtCorBΔC R235L mutant have been deposited to the Protein Data Bank (www.rcsb.org) under accession numbers 7MSU, 7M1T, and 7M1U, respectively. Source data are provided as a Source Data file. All other data are available from the corresponding author upon reasonable 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.						
\(\sum_{\text{life sciences}}\)	iences Behavioural & social sciences Ecological, evolutionary & environmental sciences					
For a reference copy of t	the document with all sections, see <u>nature.com/docu</u>	ments/nr-reporting-summary-flat.pdf				
Life sciences study design						
All studies must dis	sclose on these points even when the disc	closure is negative.				
Sample size	No statistical method were used to predetermine the sample size. Sample sizes are specified in the figure legends & Methods section.					
Data exclusions	No data was excluded.					
Replication	All biochemical assays were replicated using multiple protein preparations. All attempts of replications were successful. Number of replications are specified in the figure legends.					
Randomization	No data randomization was applied, as all data were performed with recombinant proteins.					
Blinding	The data collection/analysis were not blinded	d, as this was not applicable to this 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.						
Materials & experimental systems		nods				
n/a Involved in the study		nvolved in the study				
Antibodies		ChIP-seq				
Eukaryotic	cell lines	Flow cytometry				
Palaeontology and archaeology		MRI-based neuroimaging				
Animals and other organisms						
	Human research participants					
Clinical data						
Dual use research of concern						