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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.

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	Bruker Topspin (version 3.5, https://www.bruker.com/products/mr/nmr/nmr-software/software/topspin/overview.html?gclid=EAIaIQobChMImvnRisrR3gIVT_IRCh0G8gRzEAAYASAAEgLzcPD_BwE), TURBOMOLE (version 6.0, https://www.turbomole.org/), ADF (version 2013, https://www.scm.com/)
Data analysis	CCPN analysis (version 2.4.2, https://www.ccpn.ac.uk/v2-software/software/analysis), VMD (version 1.9.3, https://www.ks.uiuc.edu/Research/vmd/), MATLAB (version 9.6.0 (R2019a), https://www.mathworks.com/products/matlab.html), EasySpin (version 6.0.0, https://www.easyspin.org/), Pymol (version 2.4.2, https://pymol.org/2/), dmfit (version 2019, https://nmr.cemhti.cnrs-orleans.fr/dmfit/)

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 NMR and EPR spectra can be accessed at https://doi.org/10.3929/ethz-b-000501034. The following PDB structures were used in this study: 4ZC0 [https://www.rcsb.org/structure/4ZC0], 4NMN [https://www.rcsb.org/structure/4NMN], 4ESV [https://www.rcsb.org/structure/4esv], 3CMW [https://www.rcsb.org/structure/3CMW] and 3PUW [https://www.rcsb.org/structure/3PUW]. All experimental NMR parameters are provided as a Source Data file. Source data are provided with this paper. Protein resonance assignments are available from the BMRB database (www.bmrb.wisc.edu, accession code 27879).

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	No sample-size calculation was performed, since only two samples for NMR were at maximum independently prepared and analysed.
Data exclusions	No data were excluded.
Replication	1D NMR experiments were repeated before measuring 2D spectra to check the sample stability. The NMR samples were at least prepared two times and the spectra were identical. For EPR, a 13C/15N labelled and unlabelled sample were studied and the spectra were, besides expected differences due to isotope labelelling, identical. We have previously demonstrated that the protein in its sedimented state is long-term stable in the NMR rotor (Wiegand T, et al. Sedimentation Yields Long-Term Stable Protein Samples as Shown by Solid-State NMR. Front Mol Biosci 7, 17 (2020).)
Randomization	Not relevant for magnetic resonance in which a bulk sample is studied.
Blinding	Not relevant for magnetic resonance in which a bulk sample is studied. The protein was studied in previous investigations (Wiegand T, et al. The conformational changes coupling ATP hydrolysis and translocation in a bacterial DnaB helicase. Nat Commun 10, 31 (2019), Wiegand T, et al. Nucleotide binding modes in a motor protein revealed by 31P- and 1H-detected MAS solid-state NMR. ChemBioChem 21, 324-330 (2020).) without ATP-mimics as a reference state. For EPR we also recorded control spectra (e.g. the buffer solution only or the protein with different ATP analogues, see Figure 2 of the present manuscript).

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
☒	☐ Human research participants
☒	☐ Clinical data
☒	☐ Dual use research of concern

Methods

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