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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 Authors & Referees 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	SerialEM 3.6.1
Data analysis	GCTF 1.06, Relion 3.0, UCSF Chimera 1.9, Coot 0.8.9, Resmap 1.1.4, Phenix 1.13, Gephi 0.9.2

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/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 cryo-EM maps of C. reinhardtii PSII-LHCII supercomplexes have been deposited in the Electron Microscopy Data Bank with accession codes EMD-9956 (C2S2M2L2) and EMD-9955 (C2S2). The structure models of C2S2M2L2 and C2S2 supercomplexes are deposited in the Protein Data Bank under accession code 6KAD and 6KAC, respectively.

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 statistical methods were used to predetermine sample size. The single particle cryoEM analysis averaged 454,678 particles for the reported C2S2 structure and 118,423 particles for the C2S2M2L2 structure. The sample size was chosen mainly based on prior experiences published in the literature.
Data exclusions	The initial cryoEM raw images are screened manually, and the exclusion criterion is based on the image quality and the degree of ice contamination through visual evaluation. The micrographs with low-resolution Thon ring profiles and severe ice contamination were excluded. For particle selection, 2D and 3D classification were carried out and the exclusion criterion is based on the quality of 2D class average images and 3D maps. The 2D and 3D classes with poorly defined internal features were excluded.
Replication	Cryo-EM image data collection of C2S2M2L2 sample were carried out three times with three different grids (n=3). For C2S2 sample, the cryo-EM data were collected with two different grids (n=2). The different cryo-EM grid samples of the same type were prepared under the same conditions and the cryo-EM micrographs are collected on the same electron microscope at the same period of time to ensure reproducibility of the cryoEM data. For the cryo-EM grids screened, three out of four (C2S2M2L2) and two out of eight (C2S2) produced high-quality images suitable for further high-resolution structure analysis. The oxygen-evolution activity of C2S2 sample was measured with five distinct samples (n=5) consecutively under the same conditions. All attempts in replication were successful.
Randomization	No randomization was required for the reported works as no allocation into experimental groups were needed. For single-particle cryoEM analysis, particles are divided into two random sets for reconstruction for estimation of the resolution via the Fourier Shell Correlation (FSC) method.
Blinding	Blinding to group allocation was not required for the reported works as no allocation into experimental groups were needed.

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
☒	☐ Animals and other organisms
☒	☐ Human research participants
☒	☐ Clinical data

Methods

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