***eLife’s* transparent reporting form**

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**Sample-size estimation**

* You should state whether an appropriate sample size was computed when the study was being designed
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This is generally not applicable to X-ray crystallography, however highly redundant data was collected as indicated in Tables 1 and 2.

**Replicates**

* You should report how often each experiment was performed
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* High-throughput sequence data should be uploaded before submission, with a private link for reviewers provided (these are available from both GEO and ArrayExpress)

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This is generally not applicable to X-ray crystallography, however all attempts at replication of the crystals were successful.

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* Statistical analysis methods should be described and justified
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* For each experiment, you should identify the statistical tests used, exact values of N, definitions of center, methods of multiple test correction, and dispersion and precision measures (e.g., mean, median, SD, SEM, confidence intervals; and, for the major substantive results, a measure of effect size (e.g., Pearson's r, Cohen's d)
* Report exact p-values wherever possible alongside the summary statistics and 95% confidence intervals. These should be reported for all key questions and not only when the p-value is less than 0.05.

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Tables 1 and 2 indicate statistics of the X-ray data.

(For large datasets, or papers with a very large number of statistical tests, you may upload a single table file with tests, Ns, etc., with reference to sections in the manuscript.)

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* Indicate how samples were allocated into experimental groups (in the case of clinical studies, please specify allocation to treatment method); if randomization was used, please also state if restricted randomization was applied
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Not applicable.

**Additional data files (“source data”)**

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* Where provided, these should be in the most useful format, and they can be uploaded as “Source data” files linked to a main figure or table
* Include model definition files including the full list of parameters used
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Please indicate the figures or tables for which source data files have been provided:

The atomic coordinates, structure factors, and NCS-improved phases have been deposited in the Protein Data Bank ([www.pdb.org](http://www.pdb.org)). To generate maps analogous to those presented in the Figures, the NCS-improved phases should be used rather than phases derived solely from the atomic coordinates. The accession numbers are: 6BBF (H206A Oraicryst), 6BBG (WT Oraicryst), 6BBH (K163W Oraicryst, I41 form), and 6BBI (K163W Oraicryst, P42212 form).