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Policy information about <u>availability of computer code</u>

Code availability statement

For all studies using custom code or mathematical algorithm that is deemed central to the conclusions, the manuscript must include a statement under the heading "Code availability" describing how readers can access the code, including any access restrictions. Code availability statements should be provided as a separate section after the data availability statement but before the References.

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Does not apply	Involved in the study
X	Macromolecular structural data
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X	Human embryos, gametes and/or stem cells
X	Human research participants
X	Clinical data
X	Archaeological, geological, and palaeontological materials

Macromolecular structural data

Policy information about special considerations for specific types of data

Validation report

We have provided an official validation report from wwPDB for all macromolecular structures studied.

Biological materials

Policy information about availability of materials

Obtaining biological materials	This study did not generate or use unique biological materials.	
We have described these re	strictions in the manuscript.	

Research animals
Policy information about studies involving animals; ARRIVE guidelines recommended for reporting animal research
Ethical compliance
We have complied with all relevant ethical regulations and include a statement affirming this in the manuscript.
Ethics committee We have disclosed the name(s) of the board and institution that approved the study protocol in the manuscript.
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Manuscripts involving the use of human embryos, gametes or stem cells must include an ethics statement that provides the following information: - The institutional and/or licensing committee(s) that approved the study protocol - Confirmation that informed consent was obtained from all recipients and/or donors of cells or tissues - The conditions for donating materials for the research
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Informed consent We have obtained informed consent from all participants and this is noted in the manuscript.
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Clinical studies
Policy information about <u>clinical studies</u>
Clinical trial registration We have provided the trial registration number from ClinicalTrials.gov or an equivalent agency in the manuscript.
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Tumor marker prognostic studies We have followed the REMARK reporting guidelines

Yes No

☐ Not a tumor marker prognostic study

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