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CASE STUDY · MARLUC SYNOPSIS

AlphaFold and the AlphaFold Protein Structure Database

IMPLEMENTED 2020 ONWARDS · HEALTH AND LIFE SCIENCES · UK · BAND C · PARTLY PROVED

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A deep learning system that predicts the 3D shape of a protein from its amino acid sequence, released as an open database with EMBL-EBI and recognised in the 2024 Nobel Prize in Chemistry.

ABOUT THIS SYNOPSIS

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Facts and figures are as reported by the sources listed below, which may be incomplete, self-reported or out of date. Check the original source before relying on any figure.

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NOTICE WORDING LAST UPDATED 16 NOVEMBER 2026

AT A GLANCE

Frontier case: AI used for a scientific, medical or engineering breakthrough. The transformation is potential and unproven; MarLuc grades what has changed in practice so far.

AI used: Deep learning models that predict protein structures (AlphaFold 2 and AlphaFold 3), shared through an open database and a web server.

Implemented: 2020 onwards. Grade: band C, Process change, Partly proved.

Headline result, as reported: Structure prediction is now a routine first step in many labs; independent analysis finds more experimental structures from users, with real limits on accuracy and on applied results

1 · The case

The facts, as reported by the 6 sources listed at the end. Where a source is silent, the field says "Not reported".

Organisation

Google DeepMind, with EMBL-EBI. Research system developed by Google DeepMind in London, released as an open database with EMBL-EBI, the European Bioinformatics Institute. Used by researchers worldwide. Canvas block: 4. Operations and process. Also 6. Data and technology, 3. Customers and proposition.

Business challenge

The challenge. Experimentally determining a protein structure often took a year or more of expensive, painstaking work, per DeepMind. Predicting a structure from the amino acid sequence had been an open problem for about 50 years.

How it was addressed. DeepMind entered AlphaFold in the CASP14 blind assessment in 2020, then released the AlphaFold Protein Structure Database with EMBL-EBI in 2021 and predictions for more than 200 million proteins in 2022. In 2024 it published AlphaFold 3, developed with Isomorphic Labs, which predicts the structure and interactions of proteins, DNA, RNA and small molecules, and opened a server for non-commercial researchers. [1] [2] [3] [4] [5] [6]

Who implemented it

In-house (In-house): Google DeepMind: Developed AlphaFold 2 and AlphaFold 3..
EMBL-EBI (University or research lab): Partnered with DeepMind to build and host the AlphaFold Protein Structure Database..
Isomorphic Labs (Industry partner): Developed AlphaFold 3 together with DeepMind, by DeepMind's account..
A research lab and a public data institute worked together; no outside consultancy or integrator is named in the sources.

Technology (SEAM pillar E)

SEAM types: T5 Custom / fine-tuned models, T8 Predictive / ML models. Deployment: Not reported. Vendors and products: Google DeepMind, AlphaFold 2, AlphaFold Protein Structure Database, AlphaFold 3, AlphaFold Server.

Where it was built in: Predictions are served as an open database built with EMBL-EBI, and AlphaFold 3 through a web server for non-commercial use; researchers use them within their own structural biology and drug discovery workflows.

What changed

Before: researchers needed months of laboratory work, or specialist computing, to get a structure. After: a predicted structure is available in a database, and independent analysis finds that researchers who build on AlphaFold 2 submit 45% to 49% more experimental structures, with more novel ones. Measured effects on output are modest and effects on applied research are mixed. [1] [2] [3] [4] [5] [6]

What it cost

Not reported

What it saved

Not reported as a cost saving. DeepMind says the database predictions would take hundreds of millions of years to solve experimentally. The Innovation Growth Lab finds a 2.5% rise in publication rates for researchers and 5.1% for laboratories. [1] [2] [3] [4] [5] [6]

Governance and control

CASP assessed the system blind, and an independent Nature Methods study tested it against experimental maps. AlphaFold 3 launched with restricted access, which Nature reported researchers criticised. Accountable owner and internal controls: Not reported.

S2 · Accountable owner · Not reported
Not reported.

A1 · Safe use · Evidenced
Nature reports that AlphaFold 3 is free for non-commercial use, with restrictions on uses such as drug development and daily limits on predictions. [6]

A2 · Human in the loop · Not reported
Not reported.

A3 · Monitoring and assurance · Evidenced
CASP is a blind assessment on recently solved structures, and an independent study compared predictions with experimental maps for 102 structures. [1] [5]

A4 · Vendor AI · Not reported
Not reported.

A5 · Agent controls · Not reported
Not reported. AlphaFold is not an agent.

A6 · Standards and regulation · Outside scrutiny (a regulator, court, auditor or similar body acted)
Nature applied its editorial policy on code availability to AlphaFold 3 and said it would update the paper once code was released; researchers wrote an open letter on reproducibility. [6]

What worked, what did not, what is unproven

WORKED

– Accuracy at CASP14: a median 92.4 GDT overall and 87.0 for the hardest targets, by DeepMind's account of the results.

– Reach: over 3 million database users in more than 190 countries by November 2025, per DeepMind; the Royal Swedish Academy of Sciences gave more than two million people in October 2024.

– Independent analysis of 5 million records finds 45% to 49% more experimental structure submissions and more novel structures among researchers building on AlphaFold 2.

– Papers linked to AlphaFold 2 are twice as likely to be cited in clinical articles, and 22.6% to 34.2% more likely to be cited by a patent, per the same analysis.

DID NOT

– Predictions often differ from experiment. In a Nature Methods study of 102 structures, the mean map-model correlation was 0.56 for AlphaFold predictions against 0.86 for deposited models, and the authors say predictions are not better representations of a crystal than deposited models.

– The Innovation Growth Lab finds only a modest rise in publication rates and says new structures are solved at lower resolution in less charted regions.

– AlphaFold 3 was published with pseudocode and not full code. Nature reported that researchers said this limits verification and reproducibility, and that use was restricted and capped daily.

UNPROVEN

– Whether the effects measured in the bibliometric analyses are caused by AlphaFold. The

– Whether AlphaFold has yet led to an approved medicine: Not reported in the sources.

– The pace and cost of drug discovery using AlphaFold 3: Not reported.

Timeline

Nov 2020 DeepMind reports a median score of 92.4 GDT at CASP14, which the CASP organisers recognise as a solution to the protein folding problem, by DeepMind's account [1]

2021 AlphaFold Protein Structure Database launched with EMBL-EBI [2]

2022 Predictions released for more than 200 million protein structures [2]

Nov 2023 Nature Methods paper compares 102 AlphaFold predictions with experimental crystallographic maps [5]

May 2024 Nature editorial notes AlphaFold 3 was published with pseudocode and not full code, and that researchers have criticised the restrictions [6]

Oct 2024 Nobel Prize in Chemistry 2024 awarded in part to Demis Hassabis and John Jumper for protein structure prediction [3]

Nov 2025 Independent analysis by the Innovation Growth Lab, supported by Google DeepMind, reports effects on research; DeepMind reports over 3 million database users [4]

2 · Grade and SEAM assessment

MarLuc's opinion, made on the evidence above. How cases are graded: marluc.co.uk/case-studies/how-we-rate

Level of change and impact

Claimed: A. Grade: C, Process change. Proof: Partly proved. Level of change: Process change.

Process change (Level 2, band C), claimed as transformation (band A). Structural biology now often starts from a predicted structure that is then tested, and independent data show more experimental structures from users. Transformation of the field is potential and unproven.

Graded C, claimed A. Predicting a structure first and testing it in the lab is now an accepted way of working, and independent data show more experimental structures from researchers who build on AlphaFold 2. The same studies show modest effects on output, mixed applied results and predictions that differ from experiment in places. A change of the whole field, and of the drugs it produces, is potential and unproven.

The SEAM view and lessons learnt

The transferable lesson is about adoption. Making outputs openly available through a database was what moved a research result into everyday practice, and the independent studies show the effect in real work. They also show the limit: predictions are hypotheses to test, so a buyer of AI output should keep the checking step, and the evidence for broad, causal change is still thin.

1. Treat model outputs as hypotheses and keep the step that tests them.
2. Publish outputs in a form people can use without specialist skills.
3. Commission independent assessment and publish its limits with the results.

Evidence

Score 3 of 4. Partly independent: a blind assessment, a peer-reviewed accuracy study in Nature Methods and a bibliometric analysis that the developer funded but did not control; usage figures are DeepMind's own.

Evaluation method. Peer-reviewed and independent studies plus company reporting: Nature Methods comparison of 102 predictions with crystallographic maps, an Innovation Growth Lab analysis of 5 million records (supported by Google DeepMind, which did not take part in the analysis), the Royal Swedish Academy of Sciences' Nobel statement, and DeepMind's own usage figures.

Sources disagree. DeepMind describes an increase of over 40% in novel experimental structure submissions; the Innovation Growth Lab report gives 45% to 49%. The Royal Swedish Academy of Sciences gave more than two million users in October 2024 and DeepMind gave over 3 million in November 2025, for different periods.

Status. Ongoing: database and server in use. Nature reported in May 2024 that DeepMind said it was working on releasing AlphaFold 3 for academic use within six months; the release is not confirmed in the sources opened.

3 · Original sources

Read these in full. To challenge a fact or a grade, use the contact form at marluc.co.uk or the link on https://marluc.co.uk/case-studies/alphafold-protein-structure-database

[1] Google DeepMind: AlphaFold, a solution to a 50-year-old grand challenge in biology (30 November 2020)
https://deepmind.google/discover/blog/alphafold-a-solution-to-a-50-year-old-grand-challenge-in-biology/

[2] Google DeepMind: AlphaFold, five years of impact (November 2025)
https://deepmind.google/blog/alphafold-five-years-of-impact/

[3] The Royal Swedish Academy of Sciences: Press release, the Nobel Prize in Chemistry 2024
https://www.nobelprize.org/prizes/chemistry/2024/press-release/

[4] Innovation Growth Lab: AI in Science, emerging evidence from AlphaFold 2 (summary report, 2025)
https://www.innovationgrowthlab.org/wp-content/uploads/2025/11/ai_in_science_af2_igl_summary.pdf

[5] Nature Methods: AlphaFold predictions are valuable hypotheses and accelerate but do not replace experimental structure determination (Terwilliger and others, 2023)
https://www.nature.com/articles/s41592-023-02087-4

[6] Nature: AlphaFold3, why did Nature publish it without its code? (editorial, May 2024)
https://www.nature.com/articles/d41586-024-01463-0

Google DeepMind, with EMBL-EBI website: https://alphafold.ebi.ac.uk

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VERSION HISTORY

v1.1 15 November 2026 Method update: standards and regulation (A6) relabelled "outside scrutiny" because the evidence is a regulator, court, auditor or similar body acting, not the organisation's own compliance.