

Egor Marin

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COVER PARAGRAPH

Scientist with strong computational and biophysical background and tendency towards writing reusable code. I have eight years of experience as a structural biology/bioinformatics scientist, with h-index of 13 and experience ranging from data processing in serial crystallography and cryoEM to wet-lab sample preparation and virtual ligand screening.

As a structural biologist, have 400+ hours of crystallography beamtime, 20+ Tb of processed crystallography data and **80 processed projects in CryoSPARC** instance that I also set up and managed for 15 users on multiple workstations and a SLURM cluster. As of January 2026, have **38 deposited PDB structures** across 16 different publications. Notably, for faster processing of the projects wrote a [web-server](#) for personalised CryoSPARC notifications.

I also have good knowledge of Linux systems, supported by 4 years of management of various workstations and servers for more than 30 users. I regularly contribute to structural biology and data science open-source (projects such as polars, MDAnalysis, reciprocalspaceship).

Now employed as Machine Learning Scientist, working on full-cycle predictive and generative model development for an antibody drug-discovery platform startup.

SELECTED PROJECTS

Scientist, Structure-function relationship of cysteinyl leukotriene receptors Sep 2017 — Sep 2020

- did last-mile crystallography service from membrane protein crystals to refined PDB structures and wrote manuscripts collaborating with multiple research groups
- publications in Nature Communications, Science Advances and Biomolecules

Structural biologist, Structural characterisation of microbial rhodopsins Sep 2020 — Sep 2023

- reconstituted membrane proteins in nanodiscs and processed cryoEM data subsequently
- publications in Nature Communications and Science Advances

Software developer, Implementation of parallel analysis in MDAnalysis May 2023 — Sep 2023

- implemented backward-compatible parallelization for the most popular molecular dynamics analysis package; continue contributing as a core developer

WORK EXPERIENCE

Machine Learning Scientist May 2024 — Present
ENPICOM B.V.
Den Bosch, Netherlands

- full-cycle ML model development: from literature survey and data collection and cleaning to reproducible training and deployment
- working with both generative and predictive models for various tasks in the antibody development field

Open-source software engineer May 2023 — September 2023
MDAnalysis via Google Summer of Code
Remote

- designed and wrote backward-compatible parallelization (dask / multiprocessing) for molecular dynamics trajectory analysis

PhD Researcher June 2021 — Dec 2023
University of Groningen
Groningen, Netherlands

- full-cycle membrane protein biochemistry: protein expression, purification, nanodisc reconstitution or crystallization
- processed cryoEM data (80 CryoSPARC projects), set up cryoEM data processing & management infrastructure
- supervised a project as a corresponding author: "[Regression-Based Active Learning for Accessible Acceleration of Ultra-Large Library Docking](#)"

Junior Research Associate March 2017 — September 2021
Moscow Institute of Physics and Technology
Moscow, Russia

- last-mile protein crystallography service: crystal harvesting, data management, synchrotron and XFEL data collection
- refined, analysed and deposited protein structures to PDB (38 structures as of September 2025)

SKILLS

- **Programming Languages:** Python, bash, Rust, C++, Typescript
- **Python:** uv/ruff/ty, pytest, hypothesis, pydantic, dask
- **Data Science:** polars, huggingface, pandas/numpy/sklearn/skrub
- **Visualization:** altair, marimo, matplotlib/seaborn/jupyter
- **Deep Learning:** pytorch, lightning, jax, mlflow
- **ML in biology:** protein language models, diffusion/discrete diffusion/flow matching, continuous diffusion models (AlphaFold/OpenFold/Boltz)
- **Structural biology:** cryoEM data processing and structure refinement, X-ray crystallography data collection, processing and refinement
- **Cheminformatics:** RDKit, polaris, molecular docking, structural bioinformatics (MDAnalysis/mdtraj/biotite)
- **Technologies:** AWS, Docker, k8s/SLURM, Modal, Airflow, Github actions

SELECTED PUBLICATIONS

For full list, see [google scholar](#).

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| Science Advances | July 2025 |
| <i>CryoRhodopsins: a comprehensive characterization of a new clade of microbial rhodopsins from cold environments</i> | |
| Pre-print on biorxiv | 29 April 2025 |
| <i>Structural basis for no retinal binding in flotillin-associated rhodopsins</i> | |
| Nature Communications | 4 October 2024 |
| <i>A subgroup of light-driven sodium pumps with an additional Schiff base counterion</i> | |
| Journal of Chemical Information and Modeling | December 2023 |
| <i>Regression-Based Active Learning for Accessible Acceleration of Ultra-Large Library Docking</i> | |
| Nature Communications Chemistry | 2 May 2023 |
| <i>Mirror proteorhodopsins</i> | |
| Nature Communications | August 2022 |
| <i>Structural basis for receptor selectivity and inverse agonism in S1P5 receptors</i> | |
| Biomolecules | December 2020 |
| <i>Structure-Based Virtual Screening of Ultra-Large Library Yields Potent Antagonists for a Lipid GPCR</i> | |
| Structural basis of ligand selectivity and disease mutations in cysteinyl leukotriene receptors | December 2019 |
| <i>Nature Communications</i> | |
| Science Advances | October 2019 |
| <i>Structure-based mechanism of cysteinyl leukotriene receptor inhibition by antiasthmatic drugs</i> | |

EDUCATION

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|---|------------------------|
| University of Groningen | 2019 — 2023 |
| PhD | Groningen, Netherlands |
| • thesis ‘On the methods of studying protein-ligand interaction dynamics’“ | |
| • methods: cryoEM, X-ray crystallography, molecular dynamics, protein biochemistry, protein biophysics | |
| • publications in JACS, Crystal Growth & Design, Journal of Cheminformatics & Modelling | |
| Moscow Institute of Physics and Technology | 2017 — 2019 |
| MSc in applied mathematics and physics | Moscow, Russia |
| • graduated <i>summa cum laude</i> | |
| Moscow Institute of Physics and Technology | 2017 — 2019 |
| BSc in applied mathematics and physics | Moscow, Russia |
| • graduated <i>magna cum laude</i> | |
| • related coursework: Calculus I-IV, Linear Algebra I-II, Complex Analysis, Differential Equations I-II, Analytical Mechanics I-II, Thermodynamics. | |

EXTRACURRICULAR ACTIVITIES

Open-source contributions

Jan 2021 — Present

- [polars](#): contributed to polars (issue [#25383](#): extending `replace_many` with `leftmost` option).
- [polars-distance](#): minor contribution to polars plugin for distance calculation
- [reciprocalspaceship](#): wrote parser for serial crystallography data into binary dataframe-like class

MDAnalysis Core Developer

February 2025 — Present

[MDAnalysis Core Developer](#)

- wrote a [parallel backend](#) for all analysis classes (dask/multiprocessing)
- added a [DSSP module](#) for native secondary structure assignment
- currently working on fast unified [MMCIF parser](#) based on `gemmi`

Self-hosting

Jan 2021 — Present

- self-hosting multiple applications (vikunja, llama.cpp wrappers, openwebui) for family use under a Tailscale VPN

Data Science Competitions

2018 — Present

- top-10% in Kaggle “Predict Molecular Properties” (public notebooks + gradient boosting on self-written rotationally invariant features)
- top-1 in first round of “Learning How To Smell” at AIcrowd
- top-10% in Takeda competition at Signate
- 5th place in Tochka Bank graph ML competition