

Summary of integrative structure determination of Deep learning enables the atomic structure determination of the Fanconi Anemia core complex from cryoEM (PDB ID: 9A0J, PDB-Dev ID: PDBDEV 00000055)

[illegible]

[Datasets used for modeling](#)

- De Novo model, Zenodo: [10.5281/zenodo.3979898](https://zenodo.org/record/10.5281/zenodo.3979898)
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- 3DEM volume, EMDB: [EMD-10291](https://www.ebi.ac.uk/EMDB/entry/EMD-10291)
- 3DEM volume, EMDB: [EMD-10292](https://www.ebi.ac.uk/EMDB/entry/EMD-10292)
- 3DEM volume, EMDB: [EMD-10293](https://www.ebi.ac.uk/EMDB/entry/EMD-10293)
- Crosslinking-MS data, PRIDE: [PXD014282](https://www.ebi.ac.uk/pride/archive/projects/PXD014282)
- Comparative model, Zenodo: [10.5281/zenodo.3979898](https://zenodo.org/record/10.5281/zenodo.3979898)
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- Experimental model, PDB: [4ccg](https://www.rcsb.org/structure/4ccg)
- Experimental model, PDB: [4zdt](https://www.rcsb.org/structure/4zdt)
- Experimental model, PDB: [5o6c](https://www.rcsb.org/structure/5o6c)
- Experimental model, PDB: [2d8s](https://www.rcsb.org/structure/2d8s)
- Experimental model, PDB: [1vyx](https://www.rcsb.org/structure/1vyx)
- Experimental model, PDB: [3k1l](https://www.rcsb.org/structure/3k1l)
- Experimental model, PDB: [2iqc](https://www.rcsb.org/structure/2iqc)
- Experimental model, PDB: [1r5m](https://www.rcsb.org/structure/1r5m)
- Experimental model, PDB: [5m23](https://www.rcsb.org/structure/5m23)
- Experimental model, PDB: [6chg](https://www.rcsb.org/structure/6chg)
- Experimental model, PDB: [6f9n](https://www.rcsb.org/structure/6f9n)
- Experimental model, PDB: [2pbi](https://www.rcsb.org/structure/2pbi)
- Experimental model, PDB: [5m89](https://www.rcsb.org/structure/5m89)
- Experimental model, PDB: [4ggc](https://www.rcsb.org/structure/4ggc)
- Experimental model, PDB: [6eoj](https://www.rcsb.org/structure/6eoj)
- Experimental model, PDB: [5kdo](https://www.rcsb.org/structure/5kdo)
- Experimental model, PDB: [5oql](https://www.rcsb.org/structure/5oql)
- Experimental model, PDB: [5opt](https://www.rcsb.org/structure/5opt)
- Experimental model, PDB: [3odt](https://www.rcsb.org/structure/3odt)
- Experimental model, PDB: [5a31](https://www.rcsb.org/structure/5a31)
- Experimental model, PDB: [5xyi](https://www.rcsb.org/structure/5xyi)
- Experimental model, PDB: [2ilr](https://www.rcsb.org/structure/2ilr)
- Experimental model, PDB: [5orq](https://www.rcsb.org/structure/5orq)
- Experimental model, PDB: [1fch](https://www.rcsb.org/structure/1fch)
- Experimental model, PDB: [3hym](https://www.rcsb.org/structure/3hym)

	<ul style="list-style-type: none"> - Experimental model, PDB: 3fp2 - Experimental model, PDB: 2gw1 - Experimental model, PDB: 6c9m - Experimental model, PDB: 6eou - Experimental model, PDB: 3ieg - Experimental model, PDB: 4rg9 - Experimental model, PDB: 2xpi - Experimental model, PDB: 3cyp - Experimental model, PDB: 5i9f - Experimental model, PDB: 5aio - Experimental model, PDB: 5dse - Experimental model, PDB: 4g1t - Experimental model, PDB: 4zlh - Experimental model, PDB: 2y4t - Experimental model, PDB: 3u4t - Experimental model, PDB: 4pjr - Experimental model, PDB: 4buj - 3DEM volume, Zenodo: 10.5281/zenodo.3979898
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	76, 4
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: BS3, 451 crosslinks - 1 unique EM3DRestraint: None
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 0.00 - Ramachandran outliers: 36 - Sidechain outliers: 9
Fit to data used for modeling	Satisfaction of crosslinks: 64.29%
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Name	Production sampling
2. Name	Rosetta Hybridize

Software

- [Rosetta](#) (version Rosetta version unknown:ff8ee24ee5f65423d5064cba818ede41d012:2020-08-10 10:39:53 -0700 from git@github.com:RosettaCommons/main.git)
- [trRosetta](#) (version 1.0.0)
- [HHPred](#) (version website)