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)

1. Model Composition	
Entry composition	- faap100: Chain P (888 residues) - fancL: Chain l (373 residues) - fancB: Chain b (867 residues) - fancE: Chain E (520 residues) - fancB: Chain B (867 residues) - fancC: Chain C (595 residues) - fancG: Chain g (648 residues) - fancL: Chain L (373 residues) - faap100: Chain p (888 residues) - fancF: Chain F (350 residues) - fancG: Chain G (648 residues)
	- De Novo model, File: 10.5281/zenodo.3979898 - 3DEM volume, EMDB: EMDB-10291 - 3DEM volume, EMDB: EMDB-10292 - 3DEM volume, EMDB: EMDB-10293 - Crosslinking-MS data, Linker name and number of cross-links: BS3, 451 cross-links - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available

Datasets used for modeling	- Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 4ccg - Experimental model, PDB ID: 4zdt - Experimental model, PDB ID: 5o6c - Experimental model, PDB ID: 2d8s - Experimental model, PDB ID: 1vyx - Experimental model, PDB ID: 3k1l - Experimental model, PDB ID: 2iqc - Experimental model, PDB ID: 1r5m - Experimental model, PDB ID: 5m23 - Experimental model, PDB ID: 6chg - Experimental model, PDB ID: 6f9n - Experimental model, PDB ID: 2pbi - Experimental model, PDB ID: 5m89 - Experimental model, PDB ID: 4ggc - Experimental model, PDB ID: 6eoj - Experimental model, PDB ID: 5kdo - Experimental model, PDB ID: 5oql - Experimental model, PDB ID: 5opt - Experimental model, PDB ID: 3odt - Experimental model, PDB ID: 5a31 - Experimental model, PDB ID: 5xyi - Experimental model, PDB ID: 2ilr - Experimental model, PDB ID: 5orq - Experimental model, PDB ID: 1fch - Experimental model, PDB ID: 3hym - Experimental model, PDB ID: 3fp2 - Experimental model, PDB ID: 2gw1 - Experimental model, PDB ID: 6c9m - Experimental model, PDB ID: 6eou - Experimental model, PDB ID: 3ieg - Experimental model, PDB ID: 4rg9 - Experimental model, PDB ID: 2xpi - Experimental model, PDB ID: 3cvp - Experimental model, PDB ID: 5i9f - Experimental model, PDB ID: 5aio - Experimental model, PDB ID: 5dse - Experimental model, PDB ID: 4g1t - Experimental model, PDB ID: 4zlh - Experimental model, PDB ID: 2y4t - Experimental model, PDB ID: 3u4t - Experimental model, PDB ID: 4pjr - Experimental model, PDB ID: 4buj - 3DEM volume, File: 10.5281/zenodo.3979898
2. Representation	

Resolution	Atomic
Number of rigid bodies, flexible units	76, 4
Rigid bodies	- B: 378-434, 1-370, 441-780, 231-365, 441-660, 651-770, 1-235, 466-626 - b: 378-434, 1-370, 441-780, 231-365, 441-660, 651-770, 1-235, 466-626 - C: 331-570, 176-335, 1-335, 1-175 - E: 266-520, 1-150, 261-520 - F: 140-341 - G: 44-645, 1-320, 181-320, 201-435, 204-315, 1-175, 321-648 - g: 44-645, 1-320, 181-320, 201-435, 204-315, 1-175, 321-648 - L: 191-300, 301-373, 104-373, 101-300, 2-91, 101-205, 1-100 - l: 191-300, 301-373, 104-373, 101-300, 2-91, 101-205, 1-100 - P: 28-442, 1-300, 711-820, 1-200, 186-480, 301-480, 510-609, 491-615, 714-803, 804-888, 453-507, 491-820 - p: 28-442, 1-300, 711-820, 1-200, 186-480, 301-480, 510-609, 491-615, 714-803, 804-888, 453-507, 491-820
Flexible units	- B: 435-440 - b: 435-440 - C: - - E: 151-170 - F: 342-350 - G: - - g: - - L: - - l: - - P: - - p: -
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: BS3, 451 cross-links - 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)	Model precision can not be calculated with one structure

Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 36, Number of sidechain outliers = 9
Model quality: assessment of excluded volume	Not applicable
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
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. Method	Production sampling
Name	Monte Carlo
2. Method	Rosetta Hybridize
Name	Rosetta Hybridize
Software	- Rosetta (version Rosetta version unknown:ff8ee24ee5f65423d5064cba818ede41d012fa8 2020-08-10 10:39:53 -0700 from git@github.com:RosettaCommons/main.git) - trRosetta (version 1.0.0) - HHpred (version website)