Summary of integrative structure determination of Structure of complement C3(H2O) revealed by quantitative cross-linking/mass spectrometry and modeling (PDB ID: 8ZZL, PDB-Dev ID: PDBDEV_00000021)

1. Model Composition	
Entry composition	- beta: chain(s) A (645 residues) - alpha: chain(s) B (992 residues)
Datasets used for modeling	- Experimental model, PDB: 2A73 - Experimental model, PDB: 2I07 - Mass Spectrometry data, PRIDE: PXD003486 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.1285940
2. Representation	
Number of representations	1
Scale	Coarse-grained: 1 residue(s) per bead
Number of *rigid* and *flexible* segments	13, 12
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: BS3, 115 crosslinks
4. Validation	
Number of ensembles	4
Number of models in ensembles	200, 200, 89, 111
Number of deposited models	4
Model precision (uncertainty of models)	- 18.71, Å - 10.44, Å - 16.24, Å - 14.62, Å
Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.71-99.73%
Fit to data used for modeling	Satisfaction of crosslinks: 70.83-75.28%
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*	Sampling
Method	Replica exchange monte carlo
Number of computed models	200000
2. *Name*	Sampling
Method	Replica exchange monte carlo
Number of computed models	200000
3. *Name*	Sampling
Method	Replica exchange monte carlo
Number of computed models	200000
Software	- Integrative Modeling Platform (IMP) (version develop-0a5706e202) - IMP PMI module (version 67456c0)