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	- alpha: Chain B (992 residues) - beta: Chain A (645 residues)
Datasets used for modeling	- Experimental model, PDB ID: 2A73 - Experimental model, PDB ID: 2I07 - Mass Spectrometry data, PRIDE: PXD003486 - Crosslinking-MS data, Linker name and number of cross-links: BS3, 115 cross-links
2. Representation	
Resolution	Coarse-grained: 1, 2, 6, 9 residue(s) per bead
Number of rigid bodies, flexible units	13, 12
Rigid bodies	- A: 1-73, 80-289, 292-643 - B: 2-70, 80-96, 97-155, 158-261, 264-312, 315-457, 464-618, 621-680, 683-824, 827-992
Flexible units	- A: 74-79, 290-291, 644-645 - B: 1-1, 71-79, 156-157, 262-263, 313-314, 458-463, 619-620, 681-682, 825-826
Structural coverage (rigid bodies)	98%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: BS3, 115 cross-links
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)	18.709, Å, 10.436, Å, 16.24, Å, 14.615, 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	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*	Sampling
Name	Replica exchange monte carlo
Number of computed models	200000
2. *Method*	Sampling
Name	Replica exchange monte carlo
Number of computed models	200000
3. *Method*	Sampling
Name	Replica exchange monte carlo
Number of computed models	200000
Software	- Integrative Modeling Platform (IMP) (version develop-0a5706e202) - IMP PMI module (version 67456c0)

Fit to data used for validation — Fit of model to information not used to compute it has not been determined

5. Methodology and Software