Table S1: Summary of Integrative Structure Determination of Structure of complement C3(H2O) revealed by quantitative cross-linking/mass spectrometry and modeling (PDBDEV00000021)

1. Model Composition	
Entry composition	- beta: Chain A (645 residues) - alpha: Chain B (992 residues) - beta: Chain A (645 residues) - alpha: Chain B (992 residues) - beta: Chain A (645 residues) - alpha: Chain B (992 residues) - beta: Chain A (645 residues) - alpha: Chain B (992 residues)
Datasets used for modeling	- Experimental model, PDB ID: 2A73 - Experimental model, PDB ID: 2I07 - Mass Spectrometry data, PXD003486 - CX-MS data, Linker name: B, Number of cross-links: S
2. Representation	
Atomic structural coverage	98%
Number of rigid bodies, flexible units	13, 12
Rigid regions	- A: 1-73:Experimental model/2A73, 80-289:Experimental model/2A73, 292-643:Experimental model/2A73. - B: 2-70:Experimental model/2A73, 80-96:Experimental model/2A73, 97-155:Experimental model/2A73, 158-261:Experimental model/2A73, 264-312:Experimental model/2A73, 315-457:Experimental model/2A73, 464-618:Experimental model/2A73, 621-680:Experimental model/2A73, 683-824:Experimental model/2A73, 827-992:Experimental model/2A73.
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.
Resolution	Rigid bodies: 1 residue per bead. Flexible regions: 50 residues per bead.
3. Restraints	
Physical principles	Excluded volume and Sequence connectivity.
Experimental data	- 1 unique CrossLinkRestraint: BS3, 115 cross-links
4. Validation	
Sampling validation	1. Information related to sampling validation has not been provided

Clustering algorithm ,*clustering feature*	distance threshold-based clustering, RMSD
Number of ensembles	4
Number of models in ensembles	200, 200, 89, 111
Model precision (uncertainty of models)	18.709Å, 10.436Å, 16.24Å, 14.615Å
Quality of data	1. Quality of input data has not be assessed
Assessment of atomic regions	Not applicable
Assessment of excluded volume	1. Model-1: Number of violations-3677.0 2. Model-2: Number of violations-3514.0 3. Model-3: Number of violations-3754.0 4. Model-4: Number of violations-3684.0
Fit of the model to information used to compute it	1. Fit of model to information used to compute it has not been determined
Fit of the model to information not used to compute it	1. Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
Method	Sampling
Name	Replica exchange Monte Carlo
Details	- Method details unspecified
Software	- Integrative Modeling Platform (IMP) (version develop-0a5706e202) - IMP PMI module (version 67456c0) - No location specified