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	- 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, PXD003486 - CX-MS data, Linker name and number of cross-links: BS3, 115 cross-links
2. Representation	
Atomic structural coverage	98%
Number of rigid bodies, flexible units	13, 12
Rigid bodies	- 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: N/A
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: BS3, 115 cross-links
4. Validation	
Sampling validation	- Information related to sampling validation has not been provided
Clustering algorithm ,*clustering feature*	Distance threshold-based clustering used if ensembles are deposited, 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	- Quality of input data has not be assessed
Model quality: assessment of atomic segments	Not applicable
Model quality: assessment of excluded volume	- Model-1: Number of violations-3677.0 - Model-2: Number of violations-3514.0 - Model-3: Number of violations-3754.0 - Model-4: Number of violations-3684.0
Fit of the model to information used to compute it	- CX-MS Fit of medioid: model # 1, percentage satisfied 80.87% - CX-MS Fit of medioid: model # 2, percentage satisfied 89.66% - CX-MS Fit of medioid: model # 3, percentage satisfied 83.48% - CX-MS Fit of medioid: model # 4, percentage satisfied 84.35%
Fit of the model to information not used to compute it	- 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