Full wwPDB Integrative Structure Validation Report

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PDB ID	*PDBDEV00000021*
Molecule Name	Structure of complement C3(H2O) revealed by quantitative cross-linking/mass spectrometry and modeling
Title	Structure of Complement C3(H2O) Revealed By Quantitative Cross-Linking/Mass Spectrometry And Modeling.
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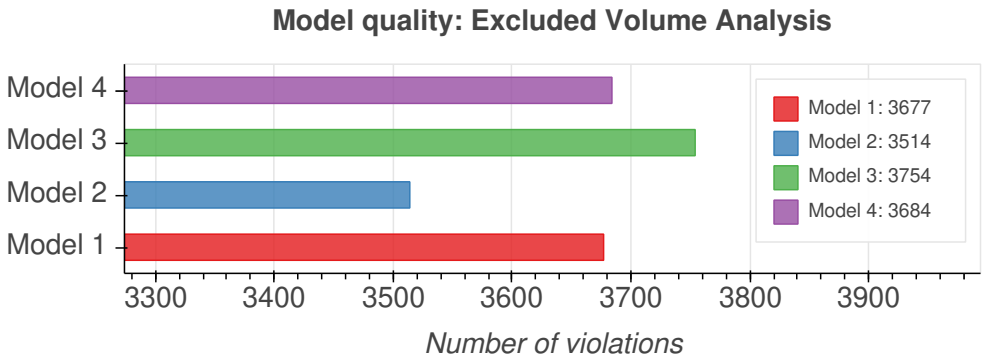
The following software were used in the production of this report:

Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance



2. Ensemble information

This entry consists of 4 distinct ensembles.

Ensemble number	*Ensemble name*	*Model ID*	*Number of models*	*Clustering method*	*Clustering feature*	*Cluster precision*
1	C3 cluster 1	1	200	None	RMSD	18.709

2	C3b cluster 1	2	200	None	RMSD	10.436
3	iC3 cluster 1	3	89	None	RMSD	16.24
4	iC3 cluster 2	4	111	None	RMSD	14.615

3. Model composition

3.1 Summary

This entry consists of 4 unique models, with 2 subunits in each model. A total of 4 datasets or restraints was used to build this entry. Each model is represented by 13 rigid bodies and 12 flexible or non-rigid units.

3.2 Entry composition

There are 4 unique types of models in this entry.These models are titled C3 cluster 1/Best scoring model, C3b cluster 1/Best scoring model, iC3 cluster 1/Best scoring model, iC3 cluster 2/Best scoring model respectively.

Model ID	*Subunit number*	*Subunit ID*	*Subunit name*	*Chain ID*	*Total residues*
1	1	1	beta	A	645
1	2	2	alpha	B	992
2	1	1	beta	A	645
2	2	2	alpha	B	992
3	1	1	beta	A	645
3	2	2	alpha	B	992
4	1	1	beta	A	645
4	2	2	alpha	B	992

3.3 Datasets used for modeling

There are 4 unique datasets used to build the models in this entry.

ID	*Dataset type*	*Database name*	*Data access code*
1	Experimental model	PDB	2A73
2	Experimental model	PDB	2I07
3	Mass Spectrometry data	PRIDE	PXD003486
4	CX-MS data	Not listed	None

4. Representation

This entry has only one representation and includes 13 rigid bodies and 12 flexible units.

Chain ID	*Rigid bodies*	*Non-rigid segments*
A	1-73:Experimental model/2A73, 80-289:Experimental model/2A73, 292-643:Experimental model/2A73.	74-79, 290-291, 644-645.
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.	1-1, 71-79, 156-157, 262-263, 313-314, 458-463, 619-620, 681-682, 825-826.

5. Methodology and software

Step number	*Protocol ID*	*Method name*	*Method type*	*Number of computed models*	*Multi state modeling*	*Multi scale modeling*
1	1	Replica exchange monte carlo	Sampling	200000	False	True
1	2	Replica exchange monte carlo	Sampling	200000	False	True
1	3	Replica exchange monte carlo	Sampling	200000	False	True

There are 2 software packages reported in this entry.

ID	*Software name*	*Software version*	*Software classification*	*Software location*
1	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building	https://integrativemodeling

2	IMP PMI module	67456c0	integrative model building	https://integrativemodeling

6. Data quality

7. Model quality

7.1 Excluded volume satisfaction

Excluded volume satisfaction for the models in the entry are listed below.

Models	***Excluded Volume Satisfaction***	***Number of violations***
1	99.73	3677
2	99.71	3514
3	99.72	3754
4	99.72	3684

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model