Full wwPDB Integrative Structure Validation Report

September 06, 2019 -- 02:06 PM

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

Integrative Modeling Package : Version XX
Molprobity : Version XX
Phenix : Version XX
Integrative Modeling Validation Package : Version XX

1. Overall quality at a glance

2. Entry composition

There is 1 unique type of model in this entry. Model has 2 chains respectively.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	beta	A	645
1	alpha	B	992

There are 2 software packages reported in this entry.

ID	Software Name	Software Version	Software Classification
1	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building
2	IMP PMI module	67456c0	integrative model building

There are 4 unique datasets used to build the model 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

3. Data quality

4. Model quality

4.1 Too-close contacts

4.2 Torsion angles

4.2.1 Protein backbone

4.2.2 Protein sidechains

5. Fit of model and data

6. Uncertaintiy of model