

# Full wwPDB Integrative Structure Validation Report

August 20, 2019 -- 05:25 PM

PDB ID	PDBDEV00000004
Molecule Name	Structure of K63-linked Diubiquitin
Title	Characterizing Protein Dynamics with Integrative Use of Bulk and Single-Molecule Techniques
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**The following softwares were used in the production of this report:**

*Integrative Modeling Package : Version XX*  
*Molprobrity : Version XX*  
*Phenix : Version XX*  
*Integrative Modeling Validation Package : Version XX*

## 1. Overall quality at a glance

## 2. Entry composition

There are 2 unique types of models in this entry. The entry contains 2 chains.

Molecule ID	Molecule Name	Chain ID	Total Residues
1	Ubiquitin	A	76
1	Ubiquitin	B	76

Software packages used for modeling were either not reported or not used.

There are 5 unique datasets used to build the model(s) in this entry.

ID	Dataset Type	Database Name	Data Access Code
1	SAS data	SASBDB	SASDCG7
2	Experimental model	PDB	1UBQ
3	Experimental model	PDB	2N2K
4	CX-MS data	Not Listed	None
5	Single molecule FRET data	Not Listed	None

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### **3. Data quality**

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### **4. Model quality**

#### **4.1 Too-close contacts**

#### **4.2 Torsion angles**

##### **4.2.1 Protein backbone**

##### **4.2.2 Protein sidechains**

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### **5. Fit of model and data**

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### **6. Uncertainty of model**

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