Full wwPDB Integrative Structure Validation Report

November 07, 2019 -- 03:08 PM

PDB ID	***PDBDEV00000022***
Molecule Name	Structural dynamics of the E6AP/UBE3A-E6-p53 enzyme-substrate complex
Title	Structural dynamics of the E6AP/UBE3A-E6-p53 enzyme-substrate complex
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The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance

2. Ensemble information

This entry consists of 1 distinct ensemble.

Ensemble number	***Ensemble name***	***Model ID***	***Number of models***	***Clustering method***	***Clustering feature***	***Cluster precision***

1	E6 main cluster	1	500	Other	RMSD	None

3. Model composition

3.1 Summary

This entry consists of 1 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 2 rigid bodies and 0 flexible or non-rigid units.

3.2 Entry composition

There is 1 unique type of model in this entry.This model is titled E6AP E6/None respectively.

Model ID	*Subunit number*	*Subunit ID*	*Subunit name*	*Chain ID*	*Total residues*
1	1	1	E6AP HECT Domain	A	350
1	2	2	E6	B	143

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	CX-MS data	Not listed	None
2	Comparative model	Not listed	None
3	Experimental model	PDB	1C4Z
4	Experimental model	PDB	4XR8

4. Representation

This entry has only one representation and includes 2 rigid bodies and 0 flexible units.

Chain ID	*Rigid bodies*	*Non-rigid segments*
A	497-846:Comparative model/None.	-
B	1-143:Comparative model/None.	-

5. Methodology and software

Step number	*Protocol ID*	*Method name*	*Method type*	*Number of computed models*	*Multi state modeling*	*Multi scale modeling*
1	1	IMP	MC based Bayesian sampling using crosslinks	720000	False	False

There is 1 software package reported in this entry.

ID	*Software name*	*Software version*	*Software classification*	*Software location*
1	Integrative Modeling Platform (IMP)	git checkout 2018/01/08 (commit 5eb8151c651256d50bbcd847932bc913df94090c)	integrative model building	https://integrativemodeling

6. Data quality

7. Model quality

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model