

Full wwPDB Integrative Structure Validation Report

August 20, 2019 -- 05:25 PM

| PDB ID | PDBDEV00000023 |
|------------------|--|
| 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 |
| Authors | Carolin Sailer;Fabian Offensperger;Alexandra Julier;Kai-Michael Kammer;Ryan Walker-Gray;Matthew G. Gold;Martin Scheffner;Florian Stengel |

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 are 1 unique types of models in this entry. The entry contains 3 chains.

| Molecule ID | Molecule Name | Chain ID | Total Residues |
|-------------|---------------------|----------|-------------------|
| 1 | E6AP HECT Domain | Α | 350 |
| 1 | E6 | В | 143 |
| 1 | p53 | С | 199 |

There are 1 software packages reported in this entry.

| ID | Software Name | Software Version | Software Classification |
|----|----------------------|---|----------------------------|
| 1 | Integrative Modeling | git checkout 2018/01/08 (commit | integrative |
| | Platform (IMP) | 5eb8151c651256d50bbcd847932bc913df94090c) | model building |

There are 4 unique datasets used to build the model(s) 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 |

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