



# Full wwPDB Integrative Structure Validation Report

November 07, 2019 -- 03:08 PM

| <i>PDB ID</i> | <i>PDBDEV00000023</i>  |
|---------------|--|
| 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       | Carolyn Sailer;Fabian Offensperger;Alexandra Julier;Kai-Michael Kammer;Ryan Walker-Gray;Matthew G. Gold;Martin Scheffner;Florian Stengel |

The following software were used in the production of this report:

*Molprobit* : 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.*

| <i>Ensemble number</i> | <i>Ensemble name</i> | <i>Model ID</i> | <i>Number of models</i> | <i>Clustering method</i> | <i>Clustering feature</i> | <i>Cluster precision</i> |
|------------------------|----------------------|-----------------|-------------------------|--------------------------|---------------------------|--------------------------|
|------------------------|----------------------|-----------------|-------------------------|--------------------------|---------------------------|--------------------------|

|   |                            |   |     |       |      |      |
|---|----------------------------|---|-----|-------|------|------|
| 1 | E6 and p53<br>main cluster | 1 | 500 | Other | RMSD | None |
|---|----------------------------|---|-----|-------|------|------|

### 3. Model composition

#### 3.1 Summary

*This entry consists of 1 unique models, with 3 subunits in each model. A total of 4 datasets or restraints was used to build this entry. Each model is represented by 3 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 p53/None respectively.*

| <i>Model ID</i> | <i>Subunit number</i> | <i>Subunit ID</i> | <i>Subunit name</i> | <i>Chain ID</i> | <i>Total residues</i> |
|-----------------|-----------------------|-------------------|---------------------|-----------------|-----------------------|
| 1               | 1                     | 1                 | E6AP HECT Domain    | A               | 350                   |
| 1               | 2                     | 2                 | E6                  | B               | 143                   |
| 1               | 3                     | 3                 | p53                 | C               | 199                   |

#### 3.3 Datasets used for modeling

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

| <i>ID</i> | <i>Dataset type</i> | <i>Database name</i> | <i>Data access code</i> |
|-----------|---------------------|----------------------|-------------------------|
| 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 3 rigid bodies and 0 flexible units.*

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

|   |                                |   |
|---|--------------------------------|---|
| C | 94-292:Comparative model/None. | - |
|---|--------------------------------|---|

## 5. Methodology and software

| <i>Step number</i> | <i>Protocol ID</i> | <i>Method name</i> | <i>Method type</i>                          | <i>Number of computed models</i> | <i>Multi state modeling</i> | <i>Multi scale modeling</i> |
|--------------------|--------------------|--------------------|---|----------------------------------|-----------------------------|-----------------------------|
| 1                  | 1                  | IMP                | MC based Bayesian sampling using crosslinks | 720000                           | False                       | False                       |

*There is 1 software package reported in this entry.*

| <i>ID</i> | <i>Software name</i>                | <i>Software version</i>   | <i>Software classification</i> | <i>Software location</i>  |
|-----------|-------------------------------------|---|--------------------------------|---|
| 1         | Integrative Modeling Platform (IMP) | git checkout 2018/01/08 (commit 5eb8151c651256d50bbcd847932bc913df94090c) | integrative model building     | <a href="https://integrativemodeling.org">https://integrativemodeling.org</a> |

## 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