# Integrative Structure Validation Report July 22, 2024 - 03:47 PM PDT

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

Python-IHM Version 1.3 MolProbity Version 4.5.2 Integrative Modeling Validation Version 1.2

PDB ID	8ZZM					
PDB-Dev ID	PDBDEV_00000022					
Structure Title	Structural dynamics of the E6AP/UBE3A-E6-p53 enzyme-substrate complex					
Structure Authors	Carolin Sailer; Fabian Offensperger; Alexandra Julier; Kai-Michael Kammer; Ryan Walker-Gray; Matthew G. Gold; Martin Scheffner; Florian Stengel					

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

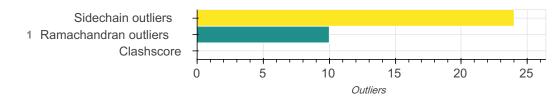
A user guide is available at https://pdb-dev.wwpdb.org/validation\_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

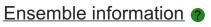
# Overall quality ?

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

#### Model Quality: MolProbity Analysis



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This entry consists of 1 distinct ensemble(s).

## Summary ?

This entry consists of 1 unique models, with 2 subunits in each model. A total of 4 datasets or restraints were used to build this entry. Each model is represented by 2 rigid bodies and 0 flexible or non-rigid units.

## Entry composition?

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

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	E6AP HECT Domain	A	A	350
1	2	2	E6	В	В	143

## 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	Crosslinking-MS data	File	10.5281/zenodo.1346675
2	Comparative model	File	10.5281/zenodo.1346675
3	Experimental model	PDB	1C4Z
4	Experimental model	PDB	4XR8

Representation ?

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

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Chain ID	Rigid bodies	Non-rigid segments
A	497-846	-
В	1-143	-

## Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	IMP	MC based Bayesian sampling using crosslinks	None	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.org

## Data quality ?

#### Crosslinking-MS

Validation for this section is under development.

# Model quality ?

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

#### Standard geometry: bond outliers?

Bond length outliers can not be evaluated for this model

Standard geometry: angle outliers?

There are 10 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be foundhere.

4 of	6
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Angle type	Observed angle (°)	ldeal angle (°)	Number of outliers
N-CA-C	111.00	88.88	1
C-N-CA	121.70	135.21	1
CA-C-N	116.20	101.40	1
O-C-N	123.00	131.68	1
N-CA-C	111.00	124.32	1
N-CA-C	111.00	97.97	1
N-CA-C	111.00	98.88	1
N-CA-C	111.00	99.23	1
N-CA-C	111.00	99.27	1
C-CA-CB	109.10	100.09	1

#### Too-close contacts?

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
1	0.00	0

All 0 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

#### Torsion angles: Protein backbone?

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	489	441	38	10

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains ?

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	449	400	25	24

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	А	500	LEU
1	А	516	ARG
1	А	592	ILE
1	А	596	LEU
1	А	613	VAL
1	А	635	LEU
1	А	642	LEU
1	А	654	MET
1	А	655	ILE
1	А	662	THR
1	А	663	ASP
1	А	678	ASP
1	А	684	ASN
1	А	685	GLU
1	А	699	LEU
1	А	706	GLN
1	А	723	LEU
1	А	728	ARG
1	А	789	THR
1	А	812	GLU
1	A	826	LEU
1	В	3	GLN
1	В	40	ARG

Model ID	Chain	Residue ID	Residue type
1	В	142	SER

# Fit of model to data used for modeling

Crosslinking-MS

Validation for this section is under development.

# Fit of model to data used for validation

Validation for this section is under development.

Acknowledgements

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