

Integrative Structure Validation Report

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

Integrative Modeling Validation Version 2.0


Python-IHM Version 1.8

MolProbity Version 4.5.2

PDB ID	8ZZM
PDB-Dev ID	PDBDEV_00000022
Structure Title	Structural dynamics of the E6AP/UBE3A-E6-p53 enzyme-substrate complex
Structure Authors	Carolyn Sailer; Fabian Offensperger; Alexandra Julier; Kai-Michael Kammer; Ryan Walker-Gray; Matthew G. Gold; Martin Scheffner; Florian Stengel
Deposited on	2018-05-30

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

We welcome your comments at helpdesk@pdb-ihm.org

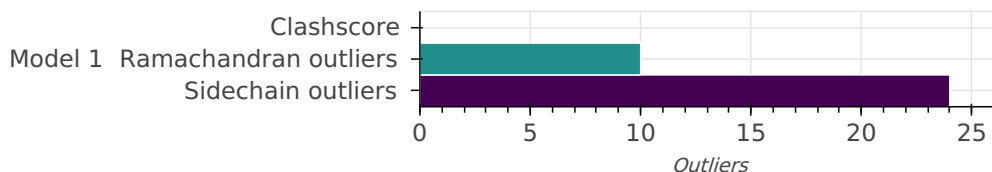
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the  symbol.

List of references used to build this report is available [here](#).

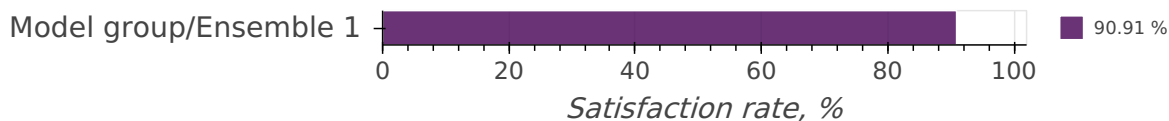
Overall quality

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS 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



Crosslink satisfaction



Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 model(s). A total of 4 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	E6AP HECT Domain	A	852	497-846	-	41.08 / 100.00	Atomic
		2	E6	B	151	1-143	-	94.70 / 100.00	Atomic

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	Zenodo	10.5281/zenodo.1346675
2	Comparative model	Zenodo	10.5281/zenodo.1346675
3	Experimental model	PDB	1C4Z
4	Experimental model	PDB	4XR8

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	MC based Bayesian sampling using crosslinks	IMP	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

At the moment, data validation is only available for crosslinking-MS data deposited as a fully [compliant](#) dataset in the [PRIDE Crosslinking](#) database. Correspondence between crosslinking-MS and entry entities is established using [pyHMMER](#). Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the [PRIDE Crosslinking](#) database.

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 ?

There are 3 bond length outliers in this entry (0.07% of 4153 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	653	MET	SD-CE	5.22	1.66	1.79	1	1
A	531	GLN	CD-NE2	4.63	1.43	1.33	1	1
A	566	MET	SD-CE	4.56	1.90	1.79	1	1

Standard geometry: angle outliers ?

There are 10 bond angle outliers in this entry (0.18% of 5593 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	745	GLN	N-CA-C	7.90	88.88	111.00	1	1
A	663	ASP	C-N-CA	7.51	135.21	121.70	1	1
A	663	ASP	CA-C-N	7.40	101.40	116.20	1	1
A	663	ASP	O-C-N	5.43	131.68	123.00	1	1
A	663	ASP	N-CA-C	4.76	124.32	111.00	1	1
A	697	TYR	N-CA-C	4.65	97.97	111.00	1	1
A	724	LYS	N-CA-C	4.33	98.88	111.00	1	1
A	818	HIS	N-CA-C	4.20	99.23	111.00	1	1
A	655	ILE	N-CA-C	4.19	99.27	111.00	1	1
A	662	THR	C-CA-CB	4.09	100.09	109.10	1	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 atomic models in this entry.

Model ID	Clash score	Number of clashes
1	0.00	0

There are no too-close contacts.

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	Analysed	Favored	Allowed	Outliers
1	489	441	38	10

There are 10 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	508	HIS	1
A	647	GLY	1
A	654	MET	1
A	664	LEU	1
A	675	GLU	1
A	698	ILE	1
A	704	GLU	1
A	727	PHE	1
A	750	THR	1
A	776	ASP	1

Torsion angles : Protein sidechains ?

In the following table, sidechain rotameric outliers are listed. The Analysed column shows the number of

residues for which the sidechain conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	449	400	25	24

There are 24 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	500	LEU	1
A	516	ARG	1
A	592	ILE	1
A	596	LEU	1
A	613	VAL	1
A	635	LEU	1
A	642	LEU	1
A	654	MET	1
A	655	ILE	1
A	662	THR	1
A	663	ASP	1
A	678	ASP	1
A	684	ASN	1
A	685	GLU	1
A	699	LEU	1
A	706	GLN	1
A	723	LEU	1
A	728	ARG	1
A	789	THR	1
A	812	GLU	1
A	826	LEU	1
B	3	GLN	1
B	40	ARG	1
B	142	SER	1

Fit of model to data used for modeling

Fit of model(s) to crosslinking-MS data

Restraint types

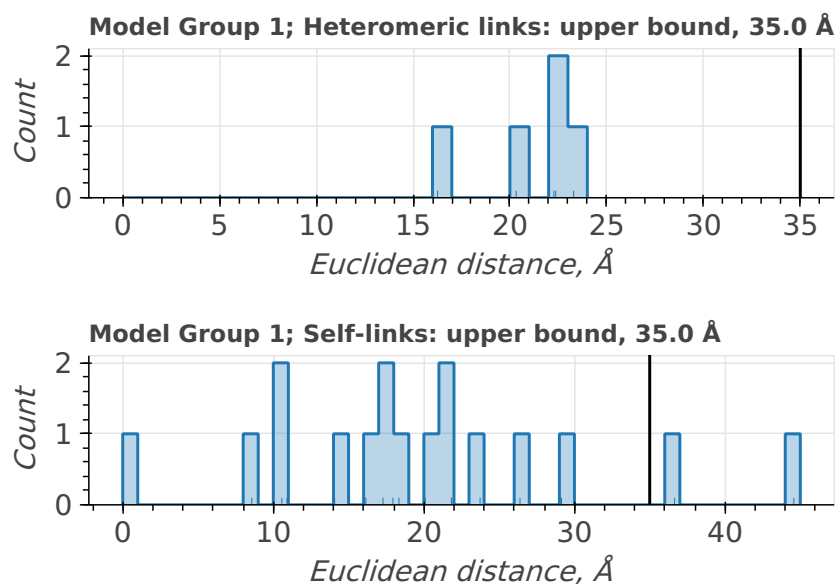
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 159 crosslinking restraints combined in 159 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSS	LYS	CA	LYS	CA	upper bound	35.0	159

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.



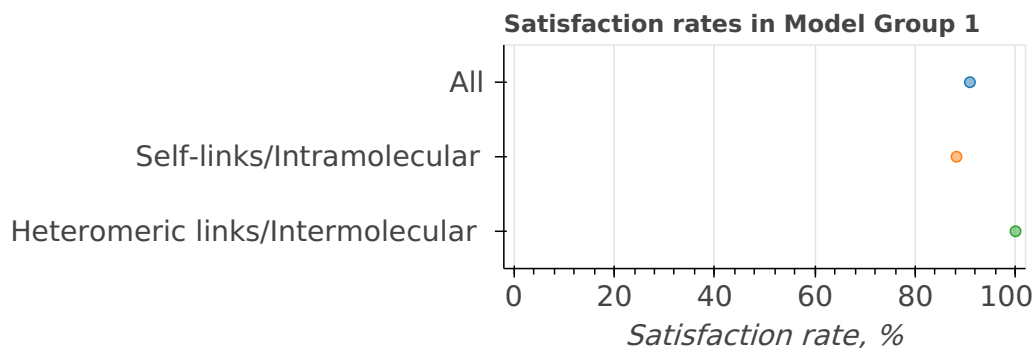
Satisfaction of restraints

Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=159)
1	1	1	1/500	All	90.91	9.09	22
				Self-links/ Intramolecular	88.24	11.76	17
				Heteromeric links/ Intermolecular	100.00	0.00	5

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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