

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

ATSAS Version 3.2.1 (r14885)

PDB ID	9A03
PDB-Dev ID	PDBDEV_00000039
Structure Title	Integrative model of 3' Nucleotide excision repair complex of XPA-DBD and RPA70AB
Structure Authors	Cordoba JJ; Topolska-Wos AM; Chazin WJ
Deposited on	2019-12-19

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

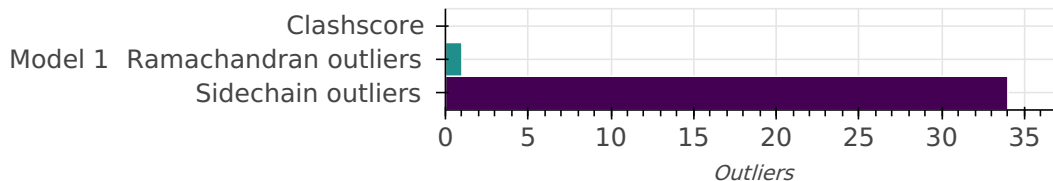
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

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



Ensemble information ?

This entry consists of 0 distinct ensemble(s).

Summary ?

This entry consists of 1 model(s). A total of 8 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	Subunit A	A	238	1-238	-	100.00 / 100.00	Atomic
		2	Subunit B	B	142	1-142	-	100.00 / 100.00	Atomic
		3	DNA short arm	C	13	1-13	-	100.00 / 0.00	Atomic
		4	DNA long arm	D	22	1-22	-	100.00 / 0.00	Atomic

Datasets used for modeling ?

There are 8 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	NMR data	BMRB	27131
2	SAS data	SASBDB	SASDH54

ID	Dataset type	Database name	Data access code
3	Experimental model	PDB	1JMC
4	Experimental model	PDB	5A39
5	Comparative model	Not available	Not available
6	Other	Not available	Not available
7	Other	Not available	Not available
None	Other	Not available	Not available

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	Homolgy Modeling of XPA	MODELLER	None	10	False	False
2	1	Extension of C-terminal Helix of XPA	ROSETTA Remodel	None	1000	False	False
3	1	Docking of DNA to XPA	HADDOCK	None	1000	False	False
4	1	Randomization and Rigid Body Energy Minimization	HADDOCK	None	1000	False	False
5	1	Semi-flexible simulated annealing	HADDOCK	None	1000	False	False
6	1	Flexible explicit solvent refinement	HADDOCK	None	200	False	False
7	1	Stepwise addition of nucleotide linker	ROSETTA stepwise	None	100	False	False

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	HADDOCK	Not available	model building	http://haddock.science.uu.nl/services/HADDOCK/
2	ROSETTA	Not available	model building	https://www.rosettacommons.org/
3	MODELLER	Not available	model building	https://salilab.org/modeller/

ID	Software name	Software version	Software classification	Software location
4	FOXS	Not available	None	https://modbase.compbio.ucsf.edu/foxs/index.html

Data quality ?

SAS:Scattering profile

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

NMR

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 ?

There are 4 bond length outliers in this entry (0.10% of 3904 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	2	DT	O3'-P	7.05	1.50	1.61	1	1
C	1	DT	O3'-P	7.03	1.50	1.61	1	1
C	3	DT	O3'-P	7.02	1.50	1.61	1	1
C	4	DT	O3'-P	4.49	1.54	1.61	1	1

Standard geometry: angle outliers ?

There are 2 bond angle outliers in this entry (0.04% of 5396 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	4	DT	C3'-O3'-P	8.12	108.02	120.20	1	1
D	15	DC	P-O5'-C5'	6.99	109.52	120.00	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

Model ID	Clash score	Number of clashes
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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	376	348	27	1

There are 1 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
B	62	GLU	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	343	264	45	34

There are 34 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	7	SER	1
A	13	SER	1
A	22	THR	1
A	29	THR	1
A	33	SER	1
A	39	LEU	1
A	41	SER	1
A	47	GLU	1
A	76	SER	1
A	82	ILE	1
A	93	ASP	1
A	103	SER	1
A	115	THR	1
A	118	PHE	1
A	130	SER	1
A	132	ASP	1

Chain	Res	Type	Models (Total)
A	148	THR	1
A	151	THR	1
A	168	ASP	1
A	169	THR	1
A	182	ASP	1
A	193	VAL	1
A	210	SER	1
A	211	VAL	1
A	215	SER	1
A	216	THR	1
A	238	GLN	1
B	14	GLU	1
B	18	SER	1
B	22	ASN	1
B	32	CYS	1
B	34	ASP	1
B	76	SER	1
B	100	GLN	1

Fit of model to data used for modeling ?

SAS data used in this integrative model could not be validated as the sascif file is currently unavailable.

NMR

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

The development of integrative model validation metrics, implementation of a model validation

pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

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