

# Integrative Structure Validation Report ?

March 27, 2025 - 10:00 AM PDT

*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	9A04
PDB-Dev ID	PDBDEV_00000040
Structure Title	Integrative model of 5' 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](mailto:helpdesk@pdb-ihm.org)*

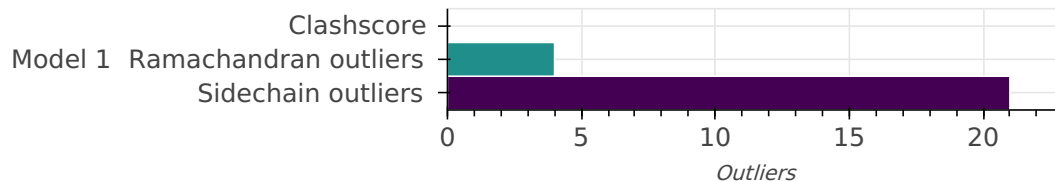
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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	14	1-14	-	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	<a href="#">27131</a>
2	SAS data	SASBDB	<a href="#">SASDH44</a>

ID	Dataset type	Database name	Data access code
3	Experimental model	PDB	<a href="#">1JMC</a>
4	Experimental model	PDB	<a href="#">5A39</a>
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	<a href="#">HADDOCK</a>	Not available	model building	<a href="http://haddock.science.uu.nl/services/HADDOCK/">http://haddock.science.uu.nl/services/HADDOCK/</a>
2	<a href="#">ROSETTA</a>	Not available	model building	<a href="https://www.rosettacommons.org/">https://www.rosettacommons.org/</a>
3	<a href="#">MODELLER</a>	Not available	model building	<a href="https://salilab.org/modeller/">https://salilab.org/modeller/</a>

ID	Software name	Software version	Software classification	Software location
4	<a href="#">FOXS</a>	Not available	None	<a href="https://modbase.compbio.ucsf.edu/foxs/index.html">https://modbase.compbio.ucsf.edu/foxs/index.html</a>

### 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 5 bond length outliers in this entry (0.13% of 3926 assessed bonds). A summary is provided below.*

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	10	DC	O3'-P	76.68	2.76	1.61	1	1
C	11	DC	O3'-P	7.07	1.50	1.61	1	1
C	12	DC	O3'-P	7.06	1.50	1.61	1	1
C	13	DC	O3'-P	6.97	1.50	1.61	1	1
C	14	DC	C3'-O3'	6.11	1.24	1.42	1	1

#### Standard geometry: angle outliers ?

*There are 4 bond angle outliers in this entry (0.07% of 5426 assessed bonds). A summary is provided below.*

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
C	10	DC	C3'-O3'-P	39.60	60.80	120.20	1	1
C	10	DC	O3'-P-O5'	33.96	53.05	104.00	1	1
D	13	DG	P-O5'-C5'	8.42	107.38	120.00	1	1
C	11	DC	P-O5'-C5'	7.01	109.49	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

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	343	29	4

There are 4 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	57	ASN	1
B	3	PHE	1
B	62	GLU	1
B	64	PRO	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	282	40	21

There are 21 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	13	SER	1
A	22	THR	1
A	33	SER	1
A	41	SER	1
A	88	THR	1
A	115	THR	1
A	130	SER	1
A	132	ASP	1
A	133	SER	1
A	148	THR	1
A	154	SER	1
A	169	THR	1

Chain	Res	Type	Models (Total)
A	182	ASP	1
A	184	ASP	1
A	214	SER	1
A	216	THR	1
A	234	ASP	1
B	15	PHE	1
B	34	ASP	1
B	55	ASP	1
B	57	ASP	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*

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