Integrative Structure Validation Report

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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	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

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

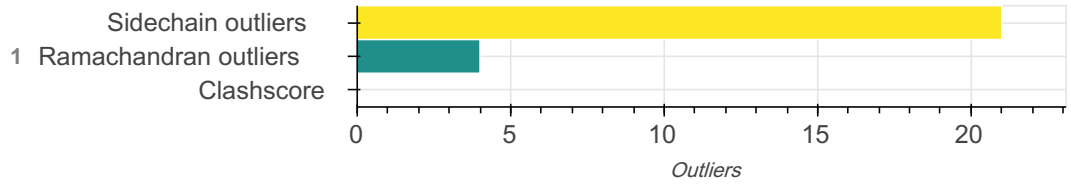
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 1 unique models, with 4 subunits in each model. A total of 8 datasets or restraints were used to build this entry. Each model is represented by 4 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 All models/Best scoring model.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Subunit A	A	A	238
1	2	2	Subunit B	B	B	142
1	3	3	DNA short arm	C	C	14
1	4	4	DNA long arm	D	D	22

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	SASDH44

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

Representation

This entry has only one representation and includes 4 rigid bodies and 0 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	1-238	-
B	1-142	-
C	1-14:None	-
D	1-22:None	-

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	MODELLER	Homolgy Modeling of XPA	None	10	False	False

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
2	1	ROSETTA Remodel	Extension of C-terminal Helix of XPA	None	1000	False	False
3	1	HADDOCK	Docking of DNA to XPA	None	1000	False	False
4	1	HADDOCK	Randomization and Rigid Body Energy Minimization	None	1000	False	False
5	1	HADDOCK	Semi-flexible simulated annealing	None	1000	False	False
6	1	HADDOCK	Flexible explicit solvent refinement	None	200	False	False
7	1	ROSETTA stepwise	Stepwise addition of nucleotide linker	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/
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

Bond length outliers can not be evaluated for this model

Standard geometry: angle outliers

Bond angle outliers do not exist or can not be evaluated for this model

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	376	343	29	4

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	343	282	40	21

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	A	2	0ASP
1	A	32	0SER

Model ID	Chain	Residue ID	Residue type
1	A	34	0THR
1	A	52	0ASP

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.

Acknowledgements

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