

Integrative Structure Validation Report ?

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

Python-IHM Version 1.3
Integrative Modeling Validation Version 1.2

PDB ID	9A0E
PDB-Dev ID	PDBDEV_00000050
Structure Title	Structural basis of CD4 downregulation by HIV-1 Nef
Structure Authors	Kwon Y; Kaake RM; Echeverria I; Suarez M; Karimian Shamsabadi M; Stoneham C; Ramirez PW; Kress J; Singh R; Sali A; Krogan N; Guatelli J; Jia X

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

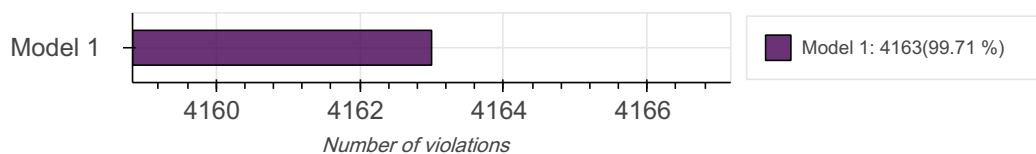
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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: Excluded Volume Analysis



Ensemble information

This entry consists of 1 distinct ensemble(s).

Summary

This entry consists of 1 unique models, with 6 subunits in each model. A total of 5 datasets or restraints were used to build this entry. Each model is represented by 11 rigid bodies and 14 flexible or non-rigid units.

Entry composition

There is 1 unique type of models in this entry. This model is titled Cluster 0 in state State_0/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Nef	A	A	242
1	2	2	CD4mut	B	B	419
1	3	3	AP2alpha2	C	C	627
1	4	4	AP2mu2	D	D	135
1	5	5	AP2sigma	E	E	142
1	6	6	AP2beta2	F	F	591

Datasets used for modeling

There are 5 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	File	10.5281/zenodo.3836213
2	Experimental model	PDB	2VGL
3	Comparative model	File	10.5281/zenodo.3836213

ID	Dataset type	Database name	Data access code
4	Mass Spectrometry data	PRIDE	PXD019338
5	Crosslinking-MS data	File	10.5281/zenodo.3836213

Representation

This entry has only one representation and includes 11 rigid bodies and 14 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	33-202	21-32, 203-222
B	405-418	394-404, 419-419
C	9-619	1-8, 620-627
D	1-124	125-135
E	1-142	-
F	15-23, 29-43, 49-61, 64-78, 81-86, 91-583	1-14, 24-28, 44-48, 62-63, 79-80, 87-90, 584-591

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	Replica exchange monte carlo	Sampling	None	2007800	False	True

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	develop-29bf2b61d4	integrative model building	https://integrativemodeling.org

ID	Software name	Software version	Software classification	Software location
2	Integrative Modeling Platform (IMP)	develop-29bf2b61d4	integrative model building	https://integrativemodeling.org
3	MODELLER	9.22	comparative modeling	https://salilab.org/modeller/

Data quality ?

Crosslinking-MS

Validation for this section is under development.

Mass Spectrometry

Validation for this section is under development.

Model quality ?

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

Excluded volume satisfaction ?

Excluded volume satisfaction for the models in the entry are listed below.

Models	Excluded Volume Satisfaction (%)	Number of violations
1	99.71	4163.0

Fit of model to data used for modeling ?

Crosslinking-MS

Validation for this section is under development.

Mass Spectrometry

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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