

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	9A1I
PDB-Dev ID	PDBDEV_00000090
Structure Title	Integrative structure determination of the A3G-CRL5-Vif complex (rigid)
Structure Authors	Robyn M Kaake; Ignacia Echeverria; Seung Joong Kim; John Von Dollen; Nicholas M Chesarino; Yuqing Feng; Clinton Yu; Hai Ta; Linda Chelico; Lan Huang; John Gross; Andrej Sali; Nevan J Krogan

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

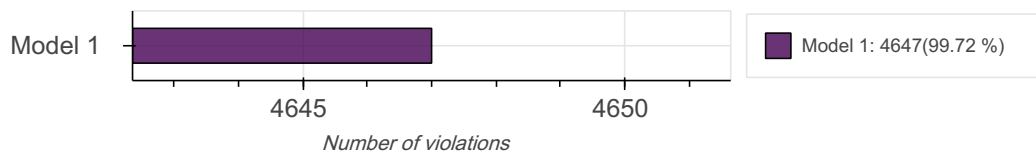
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 7 subunits in each model. A total of 11 datasets or restraints were used to build this entry. Each model is represented by 13 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	CBFB	A	A	182
1	2	2	Vif	B	B	175
1	3	3	EloB	C	C	161
1	4	4	EloC	D	D	112
1	5	5	CUL5	E	E	780
1	6	6	Rbx2	F	F	113
1	7	7	A3G	G	G	384

Datasets used for modeling

There are 11 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	4N9F
2	Experimental model	PDB	1LDJ

ID	Dataset type	Database name	Data access code
3	Experimental model	PDB	2ECL
4	Experimental model	PDB	2MA9
5	Comparative model	File	10.5281/zenodo.5176959
6	Experimental model	PDB	5K81
7	Comparative model	File	10.5281/zenodo.5176959
8	Experimental model	PDB	3V4K
9	Comparative model	File	10.5281/zenodo.5176959
10	Mass Spectrometry data	PRIDE	PXD025391
11	Crosslinking-MS data	File	10.5281/zenodo.5176959

Representation ?

This entry has only one representation and includes 13 rigid bodies and 14 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	1-156	157-182
B	6-154, 166-175	1-5, 155-165
C	1-105	106-161
D	17-112	1-16
E	11-118, 133-302, 308-382, 405-780	1-10, 119-132, 303-307, 383-404
F	27-113	1-26
G	6-194, 200-243, 258-380	1-5, 195-199, 244-257, 381-384

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	937225	False	True

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	develop-548de65454	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	develop-548de65454	integrative model building	https://integrativemodeling.org
3	MODELLER	9.20	comparative modeling	https://salilab.org/modeller/
4	MODELLER	9.19	comparative modeling	https://salilab.org/modeller/

Data quality ?

Mass Spectrometry

Validation for this section is under development.

Crosslinking-MS

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	99.72	4647.0

Fit of model to data used for modeling ?

Mass Spectrometry

Validation for this section is under development.

Crosslinking-MS

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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