

# Integrative Structure Validation Report ?

July 22, 2024 - 04:33 PM PDT

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

*Python-IHM Version 1.3*  
*Integrative Modeling Validation Version 1.2*

PDB ID	9A1J
PDB-Dev ID	PDBDEV_00000091
Structure Title	Integrative structure determination of the A3G-CRL5-Vif complex (flexible)
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](mailto:pdb-dev@mail.wwpdb.org)*

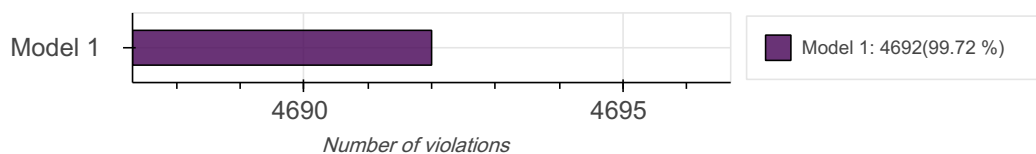
*A user guide is available at [https://pdb-dev.wwpdb.org/validation\\_help.html](https://pdb-dev.wwpdb.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

*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 12 datasets or restraints were used to build this entry. Each model is represented by 15 rigid bodies and 16 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 12 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
12	Crosslinking-MS data	File	10.5281/zenodo.5176959

## Representation

*This entry has only one representation and includes 15 rigid bodies and 16 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	11-302, 308-382, 405-515, 521-568, 574-687, 695-780	1-10, 303-307, 383-404, 516-520, 569-573, 688-694
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	203100	False	True

There are 4 software packages reported in this entry.

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

## 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, molprobability 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	4692.0

### 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*

*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 ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The [PDB-Dev team](#) and members of [Sali lab](#) contributed model validation metrics and software packages.*

*Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods.*

*Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.*