

Integrative Structure Validation Report ?

February 18, 2025 - 08:32 AM PST

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

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
Deposited on	2021-08-11

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

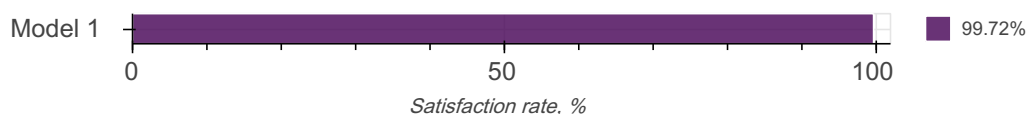
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

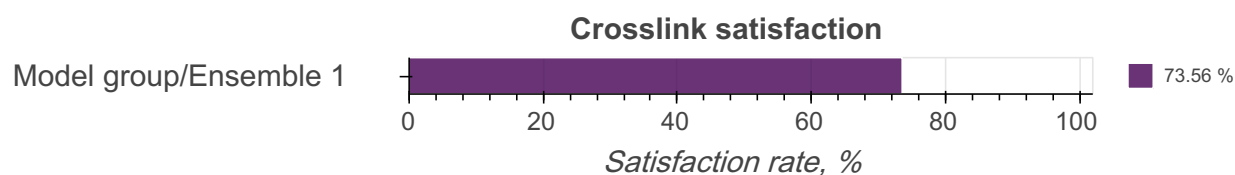
List of references used to build this report is available [here](#).

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: Excluded Volume Analysis





Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 model(s). A total of 11 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	CBFB	A	182	1-156	157-182	100.00 / 85.71	Multiscale: Coarse-grained: 1 - 5 residue(s) per bead
		2	Vif	B	175	6-154, 166-175	1-5, 155-165	100.00 / 90.86	Coarse-grained: 1 residue(s) per bead
		3	EloB	C	161	1-105	106-161	100.00 / 65.22	Multiscale: Coarse-grained: 1 - 5 residue(s) per bead
		4	EloC	D	112	17-112	1-16	100.00 / 85.71	Multiscale: Coarse-grained: 1 - 5 residue(s) per bead
		5	CUL5	E	780	11-118, 133-302, 308-382, 405-780	1-10, 119-132, 303-307, 383-404	100.00 / 93.46	Coarse-grained: 1 residue(s) per bead
		6	Rbx2	F	113	27-113	1-26	100.00 / 76.99	Multiscale: Coarse-grained: 1 - 5 residue(s) per bead

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		7	A3G	G	384	6-194, 200-243, 258-380	1-5, 195-199, 244-257, 381-384	100.00 / 92.71	Coarse-grained: 1 residue(s) per bead

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
3	Experimental model	PDB	2ECL
4	Experimental model	PDB	2MA9
5	Comparative model	Zenodo	10.5281/zenodo.5176959
6	Experimental model	PDB	5K81
7	Comparative model	Zenodo	10.5281/zenodo.5176959
8	Experimental model	PDB	3V4K
9	Comparative model	Zenodo	10.5281/zenodo.5176959
10	Mass Spectrometry data	PRIDE	PXD025391
11	Crosslinking-MS data	Zenodo	10.5281/zenodo.5176959

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	Sampling	Replica exchange monte carlo	None	937225	False	True

There are 4 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
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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 ?

Crosslinking-MS

At the moment, data validation is only available for crosslinking-MS data deposited as a fully *compliant* dataset in the *PRIDE Crosslinking* database. Correspondence between crosslinking-MS and entry entities is established using *pyHMMER*. Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the *PRIDE Crosslinking* database.

Mass Spectrometry

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.

Excluded volume satisfaction ?

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-particle or particle-atom pairs for which excluded volume was analysed.

Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
1	1638955	4647	99.72

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

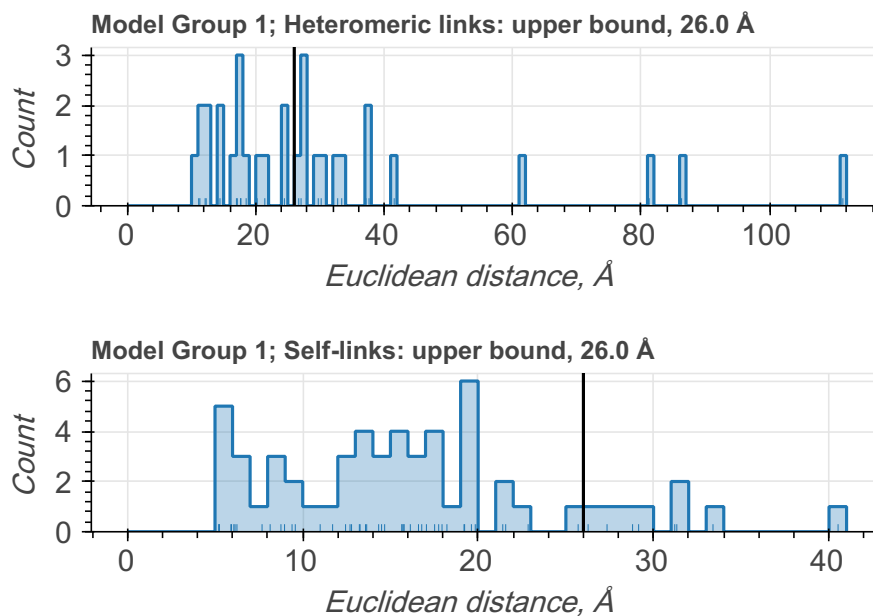
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 132 crosslinking restraints combined in 132 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSSO	LYS	CA	LYS	CA	upper bound	26.0	124
DSSO	LYS	CA	MET	CA	upper bound	26.0	7
DSSO	LYS	coarse-grained	LYS	coarse-grained	upper bound	26.0	1

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.



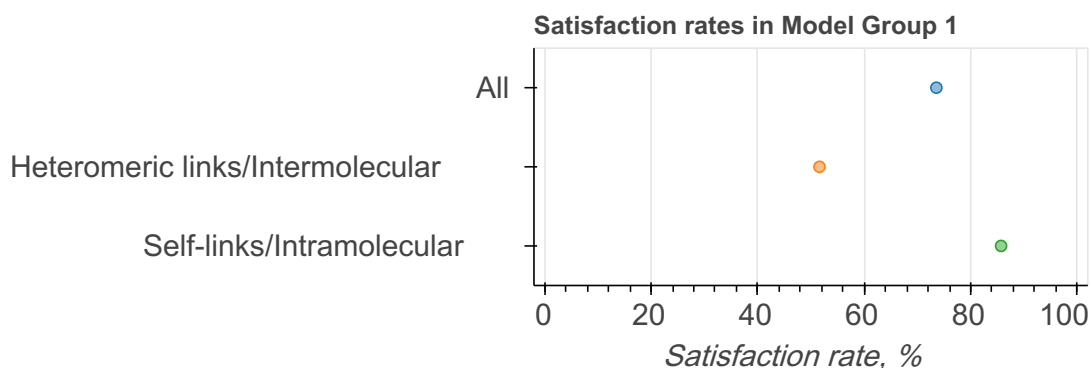
Satisfaction of restraints

Satisfaction of restraints is calculated on a *restraint group* (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (*all/any*). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=132)
1	1	1	1/857561	All	73.56	26.44	87
				Heteromeric links/ Intermolecular	51.61	48.39	31
				Self-links/ Intramolecular	85.71	14.29	56

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



Mass Spectrometry

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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