

Summary of integrative structure determination of Integrative structure determination of the A3G-CRL5-Vif complex (flexible) (PDB ID: 9A1J, PDB-Dev ID: PDBDEV_0000091)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - CFBF: chain(s) A (182 residues) - Vif: chain(s) B (175 residues) - EloB: chain(s) C (161 residues) - EloC: chain(s) D (112 residues) - CUL5: chain(s) E (780 residues) - Rbx2: chain(s) F (113 residues) - A3G: chain(s) G (384 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 4N9F - Experimental model, PDB: 1LDJ - Experimental model, PDB: 2ECL - Experimental model, PDB: 2MA9 - Comparative model, Zenodo: 10.5281/zenodo.5176959 - Experimental model, PDB: 5K81 - Comparative model, Zenodo: 10.5281/zenodo.5176959 - Experimental model, PDB: 3V4K - Comparative model, Zenodo: 10.5281/zenodo.5176959 - Mass Spectrometry data, PRIDE: PXD025391 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.5176959 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.5176959
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 5 residue(s) per bead
Number of <i>rigid</i> and <i>flexible</i> segments	15, 16
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSSO, 100 crosslinks - 1 unique CrossLinkRestraint: DSSO, 32 crosslinks
4. Validation	
Number of ensembles	1
Number of models in ensembles	198632
Number of deposited models	1

<i>Model precision (uncertainty of models)</i>	19.85, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.72%
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 81.91%
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<i>1. Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	203100
<i>Software</i>	<ul style="list-style-type: none"> - IMP PMI module (version develop-548de65454) - Integrative Modeling Platform (IMP) (version develop-548de65454) - MODELLER (version 9.20) - MODELLER (version 9.19)