

Summary of integrative structure determination of Integrative structure determination of the A3G-CRL5-Vif complex (rigid) (PDB ID: 9A1I, PDB-Dev ID: PDBDEV_00000090)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - EloC: Chain D (112 residues) - CUL5: Chain E (780 residues) - Rbx2: Chain F (113 residues) - A3G: Chain G (384 residues) - CBFB: Chain A (182 residues) - EloB: Chain C (161 residues) - Vif: Chain B (175 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB ID: 4N9F - Experimental model, PDB ID: 1LDJ - Experimental model, PDB ID: 2ECL - Experimental model, PDB ID: 2MA9 - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 5K81 - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 3V4K - Comparative model, template PDB ID: Not available - Mass Spectrometry data, PRIDE: PXD025391 - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 132 cross-links
2. Representation	
Resolution	Coarse-grained: 1, 4, 5, 6, 10, 11, 12, 14, 22 residue(s) per bead
Number of <i>rigid bodies</i>, <i>flexible units</i>	13, 14
<i>Rigid bodies</i>	<ul style="list-style-type: none"> - A: 1-156 - B: 6-154, 166-175 - C: 1-105 - D: 17-112 - E: 11-118, 133-302, 308-382, 405-780 - F: 27-113 - G: 6-194, 200-243, 258-380
<i>Flexible units</i>	<ul style="list-style-type: none"> - A: 157-182 - B: 1-5, 155-165 - C: 106-161 - D: 1-16 - E: 1-10, 119-132, 303-307, 383-404 - F: 1-26 - G: 1-5, 195-199, 244-257, 381-384
Structural coverage (<i>rigid bodies</i>)	89%
3. Restraints	

Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSSO, 132 cross-links
4. Validation	
Number of ensembles	1
Number of models in ensembles	857561
Number of deposited models	1
Model precision (uncertainty of models)	9.27, Å
Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.72-99.72%
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Method	Sampling
Name	Replica exchange monte carlo
Number of computed models	937225
Software	<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)