

Summary of integrative structure determination of model of Cullin4 (PDB ID: 9A40, PDB-Dev ID: PDBDEV_00000221)

1. Model Composition	
<u>Entry composition</u>	- G7N4W9_MACMU: Chain E (628 residues) - A4UDG5_SIV: Chain F (138 residues) - DDB1_HUMAN: Chain C (1142 residues) - CUL4A_HUMAN: Chain A (739 residues) - DCAF1_HUMAN: Chain B (373 residues) - RBX1_HUMAN: Chain D (98 residues)
<u>Datasets used for modeling</u>	Crosslinking-MS data, Linker name and number of cross-links: SDA, 1534 cross-links
2. Representation	
<u>Resolution</u>	Atomic
<u>Number of rigid bodies, flexible units</u>	0, 6
<u>Flexible units</u>	- C: 1-1142 - B: 1-373 - F: 1-138 - A: 1-739 - E: 1-628 - D: 1-98
<u>Structural coverage (rigid bodies)</u>	100%
3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	- 1 unique CrossLinkRestraint: SDA, 1534 cross-links
4. Validation	
<u>Number of ensembles</u>	0
<u>Number of models in ensembles</u>	Not applicable
<u>Number of deposited models</u>	1
<u>Model precision (uncertainty of models)</u>	Model precision can not be calculated with one structure
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of atomic segments</u>	Model-1: Clashscore = 0.32, Number of Ramachandran outliers = 20, Number of sidechain outliers = 30

<u>Model quality: assessment of excluded volume</u>	Not applicable
<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <u>Method</u>	AlphaLink2
<u>Name</u>	AlphaLink2
<u>Description</u>	No starting models were used in the modeling
<u>Number of computed models</u>	1
<u>Software</u>	AlphaLink2 (version 1.0)