

Summary of integrative structure determination of integrative threading of the dna-pkcs sequence based on data from chemical cross-linking and hydrogen deuterium exchange (PDBDEV00000034)

1. Model Composition	
Entry composition	- DNA-PKcs: Chain A (4128 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - CX-MS data, Linker name and number of cross-links: DSG, 63 cross-links - CX-MS data, Linker name and number of cross-links: DSS, 48 cross-links - CX-MS data, Linker name and number of cross-links: BSP, 52 cross-links - H/D exchange data, PXD016595 - Experimental model, PDB ID: 5LUQ
2. Representation	
Atomic structural coverage	100%
Number of rigid bodies, flexible units	1, 0
Rigid bodies	- A: 1-4128:Experimental model/5LUQ.
Flexible units	- A: -
Resolution	<ul style="list-style-type: none"> - Rigid bodies: 1 residue per bead. - Flexible regions: N/A
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSG, 63 cross-links - 1 unique CrossLinkRestraint: DSS, 48 cross-links - 1 unique CrossLinkRestraint: BSP, 52 cross-links
4. Validation	
Sampling validation	- Information related to sampling validation has not been provided
Clustering algorithm ,clustering feature	Distance threshold-based clustering used if ensembles are deposited, None
Number of ensembles	2
Number of models in ensembles	2758, 2242
Model precision (uncertainty of models)	NoneÅ, NoneÅ
Quality of data	- Quality of input data has not be assessed
Model quality: assessment of atomic segments	Not applicable

<i>Model quality: assessment of excluded volume</i>	<ul style="list-style-type: none"> - Model-1: Number of violations-0.0 - Model-2: Number of violations-0.0 - Model-3: Number of violations-0.0 - Model-4: Number of violations-0.0 - Model-5: Number of violations-0.0 - Model-6: Number of violations-0.0 - Model-7: Number of violations-0.0 - Model-8: Number of violations-0.0 - Model-9: Number of violations-0.0 - Model-10: Number of violations-0.0
<i>Fit of the model to information used to compute it</i>	<ul style="list-style-type: none"> - CX-MS Fit of medioid: model # 1, percentage satisfied 96.88% - CX-MS Fit of medioid: model # 2, percentage satisfied 96.88% - CX-MS Fit of medioid: model # 3, percentage satisfied 96.88% - CX-MS Fit of medioid: model # 4, percentage satisfied 96.88% - CX-MS Fit of medioid: model # 5, percentage satisfied 96.88% - CX-MS Fit of medioid: model # 6, percentage satisfied 96.88% - CX-MS Fit of medioid: model # 7, percentage satisfied 96.97% - CX-MS Fit of medioid: model # 8, percentage satisfied 96.88% - CX-MS Fit of medioid: model # 9, percentage satisfied 96.88% - CX-MS Fit of medioid: model # 10, percentage satisfied 96.88%
<i>Fit of the model to information not used to compute it</i>	- Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<i>Method</i>	Production sampling
<i>Name</i>	Enumeration
<i>Details</i>	- Method details unspecified
<i>Software</i>	<ul style="list-style-type: none"> - PSIPRED (version 4.0) - Integrative Modeling Platform (IMP) (version 2.2) - scikit-learn (version 0.21.3) - No location specified