



Full RCSB Integrative Structure Validation Report

March 04, 2021 -- 12:48 PM

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

Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000034
Molecule Name	Integrative threading of the DNA-PKcs sequence based on data from chemical cross-linking and hydrogen deuterium exchange
Title	SSEThread: Integrative threading of the DNA-PKcs sequence based on data from chemical cross-linking and hydrogen deuterium exchange.
Authors	Saltzberg DJ;Hepburn M;Pilla KB;Schriemer DC;Lees-Miller SP;Blundell TL;Sali A

Overall quality

Model quality: Excluded Volume Analysis



Ensemble information

This entry consists of 2 distinct ensembles.

Entry composition

There are 10 unique types of models in this entry. These models are titled Example model 0 for cluster 0, Example model 1 for cluster 0, Example model 2 for cluster 0, Example model 3 for cluster 0, Example model 4 for cluster 0, Example model 0 for cluster 1, Example model 1 for cluster 1, Example model 2 for cluster 1, Example model 3 for cluster 1, Example model 4 for cluster 1 respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	DNA-PKcs	A	4128
2	1	1	DNA-PKcs	A	4128
3	1	1	DNA-PKcs	A	4128
4	1	1	DNA-PKcs	A	4128
5	1	1	DNA-PKcs	A	4128
6	1	1	DNA-PKcs	A	4128
7	1	1	DNA-PKcs	A	4128
8	1	1	DNA-PKcs	A	4128
9	1	1	DNA-PKcs	A	4128
10	1	1	DNA-PKcs	A	4128

Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Enumeration	Production sampling	2860000	False	True

Data quality

Model quality

Excluded volume satisfaction

Excluded volume satisfaction for the models in the entry are listed below.

Models	Excluded Volume Satisfaction	Number of violations
1	100.0	0.0
2	100.0	0.0
3	100.0	0.0
4	100.0	0.0
5	100.0	0.0
6	100.0	0.0
7	100.0	0.0
8	100.0	0.0
9	100.0	0.0
10	100.0	0.0

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model