

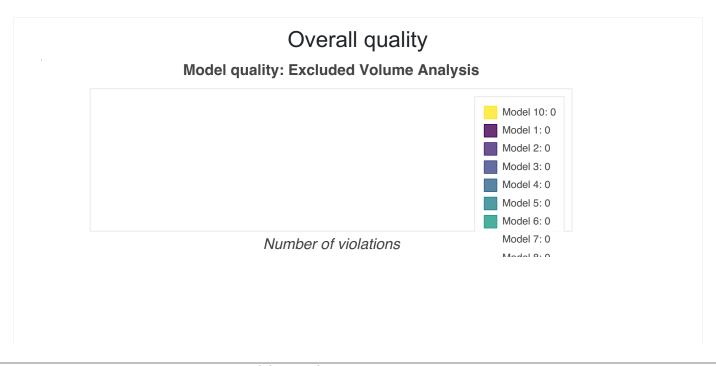
Full RCSB Integrative Structure Validation Report

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		



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 2 for cluster 1, Example model 3 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	А	4128
2	1	1	DNA-PKcs	Α	4128
3	1	1	DNA-PKcs	Α	4128
4	1	1	DNA-PKcs	Α	4128
5	1	1	DNA-PKcs	А	4128
6	1	1	DNA-PKcs	А	4128
7	1	1	DNA-PKcs	Α	4128
8	1	1	DNA-PKcs	А	4128
9	1	1	DNA-PKcs	Α	4128
10	1	1	DNA-PKcs	А	4128

Methodology and software

Step	Protocol	Method	Method	Number of computed models	Multi state	Multi scale
number	ID	name	type		modeling	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