Full RCSB Integrative Structure Validation Report

March 04, 2021 -- 12:18 PM

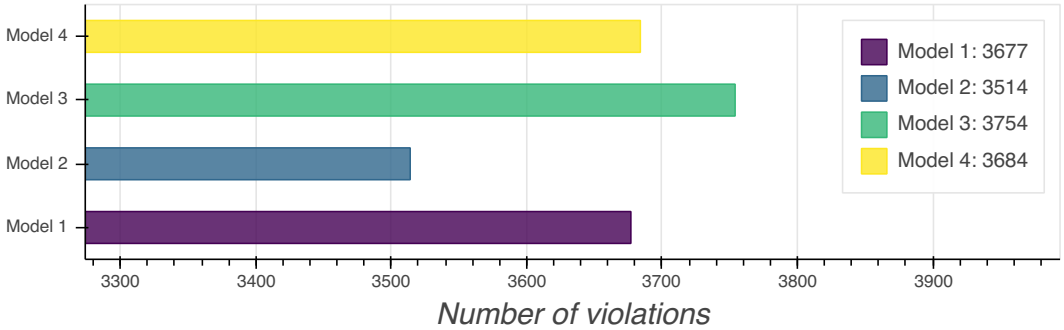
The following software were used in the production of this report:

Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000021
Molecule Name	Structure of complement C3(H2O) revealed by quantitative cross-linking/mass spectrometry and modeling
Title	Structure of Complement C3(H2O) Revealed By Quantitative Cross-Linking/Mass Spectrometry And Modeling.
Authors	Chen ZA;Pellarin R;Fischer L;Sali A;Nilges M;Barlow PN;Rappsilber J

Overall quality

Model quality: Excluded Volume Analysis



Ensemble information

This entry consists of 4 distinct ensembles.

Entry composition

There are 4 unique types of models in this entry.These models are titled C3 cluster 1/Best scoring model, C3b cluster 1/Best scoring model, iC3 cluster 1/Best scoring model, iC3 cluster 2/Best scoring model respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	beta	A	645
1	2	2	alpha	B	992
2	1	1	beta	A	645
2	2	2	alpha	B	992
3	1	1	beta	A	645
3	2	2	alpha	B	992
4	1	1	beta	A	645
4	2	2	alpha	B	992

Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Replica exchange monte carlo	Sampling	200000	True	True

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	2	Replica exchange monte carlo	Sampling	200000	True	True
1	3	Replica exchange monte carlo	Sampling	200000	True	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	99.73	3677.0
2	99.71	3514.0
3	99.72	3754.0
4	99.72	3684.0

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model