



Full wwPDB Integrative Structure Validation Report

July 06, 2020 -- 09:14 PM

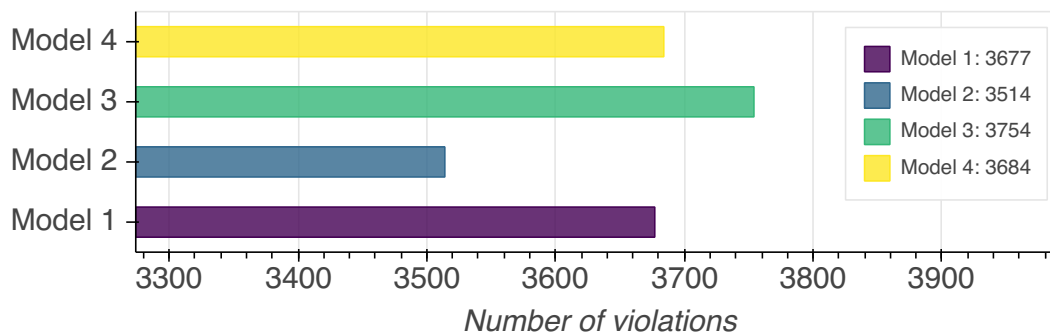
The following software were used in the production of this report:

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 |
| 1 | 2 | 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 | 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

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