Full wwPDB Integrative Structure Validation Report

July 06, 2020 -- 10:15 PM

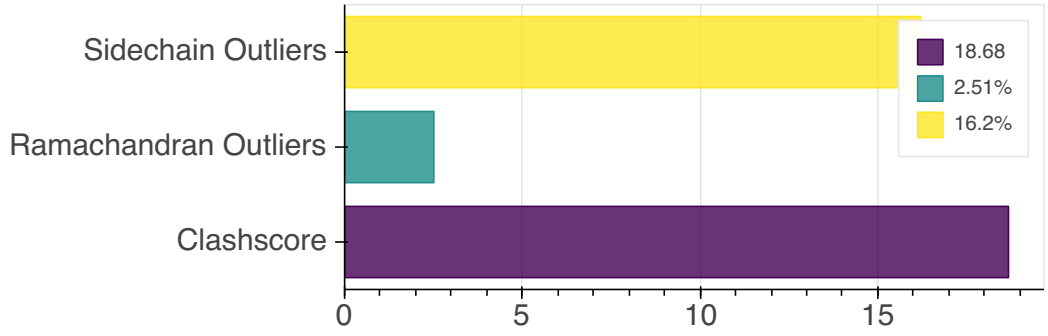
The following software were used in the production of this report:

Molprobity : Version 4.4
Integrative Modeling Validation Package : Version 1.0

PDB ID	PDBDEV_00000033
Molecule Name	Insight into the structure of the unstructured tau protein
Title	Insight into the structure of the unstructured tau protein
Authors	Popov KI;Makepeace KA;Petrotchenko EV;Dokholyan NV;Borchers CH

Overall quality

Model Quality: Molprobity Analysis



Ensemble information

This entry consists of 0 distinct ensemble.

Summary

This entry consists of 1 unique models, with 1 subunits in each model. A total of 3 datasets or restraints was used to build this entry. Each model is represented by 0 rigid bodies and 1 flexible or non-rigid units.

Entry composition

There is 1 unique type of model in this entry.This model is titled None/Best scoring model respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Total residues
1	1	1	tau protein	A	441

Methodology and software

Step number	Protocol ID	Method name	Method type	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Protein folding	Discrete Molecular Dynamics	?	False	False

Data quality

Model quality

Standard geometry

There are 662 bond outliers in this entry.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
ND1--HD1	3.149	0.86	11
OG--HG	0.979	0.84	43
OH--HH	0.98	0.84	4
NH2--HH21	1.001	0.86	13
NH2--HH22	0.976	0.86	13
N--H	0.979	0.86	384
NE--HE	0.999	0.86	13
NH1--HH11	0.979	0.86	13
N--HN	0.988	0.86	11
SG--HG	1.338	1.2	1
NH1--HH12	0.989	0.86	13
NZ--HZ3	0.977	0.89	43
NZ--HZ1	0.981	0.89	43
NZ--HZ2	0.98	0.89	43

There are 24 angle outliers in this entry.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-ND1-HD1	33.005	125.35	11
CE1-ND1-HD1	41.288	125.35	11

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all the models in this entry.

Model ID	Clash score	Number of clashes
Model 1	18.68	120

All 120 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	439	358	70	11

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:16	GLY
1	A:17	THR
1	A:28	GLY
1	A:73	GLU
1	A:100	GLY
1	A:154	PRO
1	A:176	PRO
1	A:177	PRO
1	A:183	PRO
1	A:206	PRO
1	A:301	PRO

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	Favored	Allowed	Outliers
1	358	248	52	58

Detailed list of outliers are tabulated below.

Model ID	Chain and res ID	Residue type
1	A:3	GLU
1	A:20	LEU
1	A:22	ASP
1	A:25	ASP
1	A:32	HIS
1	A:39	THR
1	A:49	GLN
1	A:50	THR
1	A:51	PRO
1	A:62	GLU
1	A:64	SER
1	A:75	VAL
1	A:93	PRO
1	A:97	ILE
1	A:102	THR
1	A:109	VAL
1	A:111	THR
1	A:122	VAL
1	A:138	ASP
1	A:141	LYS
1	A:146	ASP
1	A:162	GLN
1	A:163	LYS

Model ID	Chain and res ID	Residue type
1	A:169	THR
1	A:211	ARG
1	A:212	THR
1	A:213	PRO
1	A:217	THR
1	A:221	ARG
1	A:228	VAL
1	A:231	THR
1	A:237	SER
1	A:250	MET
1	A:252	ASP
1	A:255	ASN
1	A:258	SER
1	A:264	GLU
1	A:269	GLN
1	A:275	VAL
1	A:277	ILE
1	A:278	ILE
1	A:279	ASN
1	A:280	LYS
1	A:288	GLN
1	A:291	CYS
1	A:308	ILE

Model ID	Chain and res ID	Residue type
1	A:327	ASN
1	A:328	ILE
1	A:339	VAL
1	A:356	SER
1	A:361	THR
1	A:370	LYS
1	A:393	VAL
1	A:394	TYR
1	A:396	SER
1	A:412	SER
1	A:422	SER
1	A:427	THR

Fit of model to data used for modeling

Fit of model to data not used for modeling

Uncertainty of data and model