Integrative Structure Validation Report

July 22, 2024 - 03:53 PM PDT

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

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

PDB ID	8ZZX
PDB-Dev ID	PDBDEV_00000033
Structure Title	Insight into the structure of the unstructured tau protein
Structure Authors	Authors are not available

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

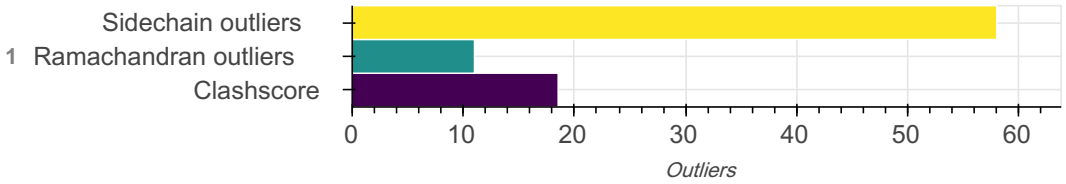
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 1 unique models, with 1 subunits in each model. A total of 3 datasets or restraints were 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 models in this entry. This model is titled None/Best scoring model.

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

Datasets used for modeling

There are 3 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Crosslinking-MS data	PRIDE	PXD015044
2	Other	PRIDE	PXD015044
3	Other	Not available	Not available

Representation

This entry has only one representation and includes 0 rigid bodies and 1 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	-	1-441

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Protein folding	Discrete Molecular Dynamics	None	_	False	False

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	piDMD	Not available	model building	http://www.moleculesinaction.com/pdmd.html
2	GROMACS	2018	model building	http://www.gromacs.org

Data quality

Crosslinking-MS

Validation for this section is under development.

Model quality

For models with atomic structures, molprobity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

There are 662 bond outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ3	0.98	0.89	9

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NZ--HZ2	0.98	0.89	15
NZ--HZ1	0.98	0.89	7
NZ--HZ2	0.99	0.89	12
NZ--HZ1	0.99	0.89	18
NZ--HZ3	0.99	0.89	12
NZ--HZ1	1.00	0.89	12
NZ--HZ3	1.00	0.89	15
NZ--HZ2	1.00	0.89	12
NH2--HH22	0.98	0.86	1
NZ--HZ1	1.01	0.89	5
NZ--HZ3	1.01	0.89	7
N--H	0.98	0.86	22
NZ--HZ2	1.01	0.89	3
NH1--HH11	0.98	0.86	1
N--H	0.99	0.86	67
NZ--HZ1	1.02	0.89	2
NZ--HZ2	1.02	0.89	2
N--HN	0.99	0.86	4
NH2--HH22	0.99	0.86	2
NH2--HH21	0.99	0.86	2
NZ--HZ3	1.02	0.89	1
NH1--HH12	0.99	0.86	1
N--H	1.00	0.86	102

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH2--HH22	1.00	0.86	5
SG--HG	1.34	1.20	1
NH2--HH21	1.00	0.86	1
OG--HG	0.98	0.84	6
NE--HE	1.00	0.86	1
OH--HH	0.98	0.84	1
NH1--HH12	1.00	0.86	4
NH1--HH11	1.00	0.86	3
N--HN	1.00	0.86	1
N--H	1.01	0.86	138
NH2--HH21	1.01	0.86	6
NH1--HH11	1.01	0.86	7
N--HN	1.01	0.86	5
OG--HG	0.99	0.84	12
NE--HE	1.01	0.86	8
NH2--HH22	1.01	0.86	4
OH--HH	0.99	0.84	3
NH1--HH12	1.01	0.86	7
N--H	1.02	0.86	56
OG--HG	1.00	0.84	12
NE--HE	1.02	0.86	5
NH1--HH11	1.02	0.86	3
NH2--HH21	1.02	0.86	5

Bond type	Observed distance (Å)	Ideal distance (Å)	Number of outliers
NH2--HH22	1.02	0.86	2
SG--HG	1.36	1.20	1
N--HN	1.02	0.86	2
NH1--HH12	1.02	0.86	2
OG--HG	1.01	0.84	11
OH--HH	1.01	0.84	1
OG--HG	1.02	0.84	3
ND1--HD1	3.15	0.86	3
ND1--HD1	3.16	0.86	3
ND1--HD1	3.17	0.86	1
ND1--HD1	3.18	0.86	5

Standard geometry: angle outliers

There are 101 angle outliers in this entry. A summary is provided below, and a detailed list of outliers can be found here.

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD2-NE2-CE1	109.00	35.18	1
CD2-NE2-CE1	109.00	35.45	1
CD2-NE2-CE1	109.00	35.69	1
CD2-NE2-CE1	109.00	35.72	1
CD2-NE2-CE1	109.00	35.74	1
CD2-NE2-CE1	109.00	35.75	1
CD2-NE2-CE1	109.00	35.80	1
CD2-NE2-CE1	109.00	35.84	1
CD2-NE2-CE1	109.00	35.95	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CD2-NE2-CE1	109.00	36.03	1
CD2-NE2-CE1	109.00	36.05	1
CD2-NE2-CE1	109.00	36.37	1
ND1-CE1-NE2	108.40	35.85	1
ND1-CE1-NE2	108.40	36.16	1
ND1-CE1-NE2	108.40	36.23	1
ND1-CE1-NE2	108.40	36.42	1
ND1-CE1-NE2	108.40	36.52	1
ND1-CE1-NE2	108.40	36.53	1
ND1-CE1-NE2	108.40	36.58	1
ND1-CE1-NE2	108.40	36.64	1
ND1-CE1-NE2	108.40	36.80	1
ND1-CE1-NE2	108.40	36.94	1
ND1-CE1-NE2	108.40	37.13	1
ND1-CE1-NE2	108.40	37.28	1
CG-CD2-NE2	107.20	72.66	1
CG-CD2-NE2	107.20	72.76	2
CG-CD2-NE2	107.20	72.90	1
CG-CD2-NE2	107.20	73.08	1
CG-CD2-NE2	107.20	73.35	1
CG-CD2-NE2	107.20	73.38	1
CG-CD2-NE2	107.20	73.41	1
CG-CD2-NE2	107.20	73.58	2

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CG-CD2-NE2	107.20	73.92	1
CG-CD2-NE2	107.20	74.33	1
CG-ND1-CE1	109.30	71.27	1
CG-ND1-CE1	109.30	71.63	1
CG-ND1-CE1	109.30	71.65	1
CG-ND1-CE1	109.30	71.70	1
CG-ND1-CE1	109.30	71.85	1
CG-ND1-CE1	109.30	72.02	1
CG-ND1-CE1	109.30	72.16	1
CG-ND1-CE1	109.30	72.27	1
CG-ND1-CE1	109.30	72.32	1
CG-ND1-CE1	109.30	72.54	1
CG-ND1-CE1	109.30	72.65	1
CG-ND1-CE1	109.30	73.13	1
CB-CG-CD2	131.20	119.78	1
CB-CG-CD2	131.20	120.22	1
CB-CG-CD2	131.20	120.31	1
CB-CG-CD2	131.20	120.54	1
CB-CG-CD2	131.20	121.50	1
CB-CG-CD2	131.20	122.23	1
CB-CG-CD2	131.20	122.29	1
CB-CG-CD2	131.20	122.64	1
CB-CG-CD2	131.20	122.94	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CB-CG-CD2	131.20	123.05	1
CB-CG-CD2	131.20	123.72	1
CB-CG-CD2	131.20	124.33	1
CB-CG-ND1	122.70	130.56	1
CB-CG-ND1	122.70	129.59	1
CB-CG-ND1	122.70	129.43	1
CB-CG-ND1	122.70	129.27	1
CB-CG-ND1	122.70	129.21	1
CB-CG-ND2	116.40	122.85	1
CB-CG-ND2	116.40	122.77	1
CB-CG-ND1	122.70	129.01	1
OD1-CG-ND2	122.60	118.41	1
CB-CG-ND1	122.70	128.98	1
CD1-CG-CD2	110.80	101.67	1
CB-CG-ND1	122.70	128.87	1
CG-CD-NE2	116.40	122.54	1
CD1-CG-CD2	110.80	101.84	1
CG-CD-NE2	116.40	122.50	1
CG-CD-NE2	116.40	122.43	1
CA-CB-CG	112.60	116.60	1
CE1-ND1-HD1	41.29	125.35	1
CE1-ND1-HD1	40.96	125.35	1
CE1-ND1-HD1	40.82	125.35	1

Angle type	Observed angle (°)	Ideal angle (°)	Number of outliers
CE1-ND1-HD1	40.71	125.35	1
CE1-ND1-HD1	40.61	125.35	1
CE1-ND1-HD1	40.35	125.35	1
CE1-ND1-HD1	40.33	125.35	1
CE1-ND1-HD1	39.80	125.35	1
CE1-ND1-HD1	39.76	125.35	1
CE1-ND1-HD1	39.73	125.35	1
CE1-ND1-HD1	39.62	125.35	2
CG-ND1-HD1	33.01	125.35	1
CG-ND1-HD1	32.77	125.35	1
CG-ND1-HD1	32.58	125.35	1
CG-ND1-HD1	32.41	125.35	1
CG-ND1-HD1	32.32	125.35	2
CG-ND1-HD1	32.22	125.35	1
CG-ND1-HD1	32.07	125.35	1
CG-ND1-HD1	32.05	125.35	1
CG-ND1-HD1	31.71	125.35	1
CG-ND1-HD1	31.48	125.35	1
CG-ND1-HD1	31.00	125.35	1

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 ID	Clash score	Number of clashes
1	18.53	119

All 119 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:229:VAL:HG12	A:399:VAL:HB	1.081
1	A:35:GLN:H	A:39:THR:HG22	0.916
1	A:234:LYS:HG2	A:405:PRO:HB3	0.912
1	A:346:PHE:HB3	A:352:SER:HB2	0.896
1	A:169:THR:HG22	A:173:ALA:HA	0.889
1	A:373:THR:HG22	A:384:ALA:H	0.880
1	A:169:THR:HG21	A:174:LYS:H	0.866
1	A:23:ARG:HD2	A:93:PRO:HB3	0.845
1	A:92:GLN:H	A:95:THR:HG22	0.808
1	A:169:THR:CG2	A:173:ALA:HA	0.798
1	A:280:LYS:HE3	A:283:ASP:HB3	0.755
1	A:233:PRO:HA	A:403:THR:HG21	0.752
1	A:19:GLY:HA2	A:24:LYS:HB2	0.748
1	A:212:THR:HG23	A:213:PRO:N	0.743
1	A:131:SER:H	A:135:THR:CG2	0.736
1	A:284:LEU:HB3	A:423:PRO:HB3	0.733
1	A:71:THR:HA	A:265:ASN:HB3	0.723
1	A:373:THR:CG2	A:384:ALA:H	0.706
1	A:231:THR:HG22	A:401:GLY:H	0.703
1	A:57:GLU:HG3	A:426:ALA:HB2	0.695

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:419:MET:HE3	A:420:VAL:HG23	0.671
1	A:245:THR:O	A:245:THR:HG23	0.660
1	A:361:THR:HG22	A:366:GLY:HA3	0.658
1	A:111:THR:HG22	A:226:VAL:HG22	0.655
1	A:361:THR:HG23	A:363:VAL:H	0.625
1	A:35:GLN:N	A:39:THR:HG22	0.622
1	A:79:LEU:HB2	A:315:LEU:HD11	0.611
1	A:427:THR:HG23	A:429:ALA:H	0.607
1	A:34:ASP:HB3	A:437:ALA:HB3	0.599
1	A:357:LEU:HB2	A:370:LYS:HG3	0.598
1	A:363:VAL:HG21	A:408:LEU:HG	0.594
1	A:352:SER:HA	A:376:LEU:HD23	0.579
1	A:123:THR:HB	A:214:SER:HB2	0.575
1	A:169:THR:O	A:169:THR:HG22	0.569
1	A:275:VAL:HG13	A:344:LEU:HG	0.559
1	A:351:GLN:H	A:377:THR:CG2	0.556
1	A:386:THR:HB	A:388:HIS:CE1	0.556
1	A:200:PRO:HB3	A:215:LEU:HD12	0.549
1	A:386:THR:HB	A:388:HIS:HE1	0.547
1	A:110:ASP:HB3	A:224:LYS:HD2	0.546
1	A:166:ALA:HB3	A:183:PRO:HD3	0.544
1	A:10:VAL:HG23	A:157:ALA:HB1	0.543
1	A:182:PRO:HG3	A:188:PRO:HG3	0.543

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:351:GLN:H	A:377:THR:HG23	0.537
1	A:427:THR:HG23	A:429:ALA:N	0.536
1	A:131:SER:H	A:135:THR:HG22	0.534
1	A:420:VAL:HG13	A:434:ALA:HB1	0.530
1	A:69:THR:HG22	A:71:THR:O	0.529
1	A:234:LYS:H	A:403:THR:HG21	0.527
1	A:29:TYR:HB2	A:46:SER:HB3	0.525
1	A:9:GLU:HB3	A:157:ALA:HB3	0.514
1	A:101:THR:HG22	A:394:TYR:O	0.514
1	A:14:HIS:HD2	A:91:ALA:O	0.514
1	A:436:LEU:HB3	A:438:LYS:HG3	0.512
1	A:212:THR:HG23	A:214:SER:H	0.511
1	A:63:THR:HG22	A:65:ASP:O	0.510
1	A:197:TYR:CE1	A:203:PRO:HG3	0.504
1	A:211:ARG:HG3	A:215:LEU:HD11	0.501
1	A:378:PHE:CD1	A:379:ARG:HB2	0.499
1	A:424:GLN:NE2	A:428:LEU:HD21	0.496
1	A:160:PRO:HB2	A:394:TYR:HB2	0.493
1	A:79:LEU:HD22	A:315:LEU:HD11	0.486
1	A:111:THR:HG21	A:150:LYS:NZ	0.483
1	A:344:LEU:O	A:353:LYS:HA	0.483
1	A:35:GLN:H	A:39:THR:CG2	0.482
1	A:277:ILE:HG21	A:280:LYS:HD2	0.481

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:288:GLN:HA	A:424:GLN:CB	0.481
1	A:288:GLN:HA	A:424:GLN:HB2	0.479
1	A:244:GLN:O	A:249:PRO:HA	0.477
1	A:310:TYR:CG	A:315:LEU:HD13	0.477
1	A:94:HIS:HD2	A:259:LYS:O	0.477
1	A:361:THR:CG2	A:366:GLY:HA3	0.474
1	A:6:GLN:HB2	A:390:ALA:O	0.472
1	A:75:VAL:HG13	A:309:VAL:HG22	0.470
1	A:386:THR:O	A:386:THR:HG23	0.468
1	A:95:THR:CG2	A:95:THR:O	0.466
1	A:52:THR:O	A:52:THR:HG23	0.465
1	A:340:LYS:HD2	A:358:ASP:HB3	0.465
1	A:34:ASP:HA	A:39:THR:HG22	0.461
1	A:102:THR:HG23	A:104:GLU:H	0.461
1	A:420:VAL:CG1	A:434:ALA:HB1	0.460
1	A:424:GLN:HE21	A:428:LEU:HD21	0.459
1	A:147:GLY:HA2	A:151:ILE:HA	0.456
1	A:231:THR:HA	A:232:PRO:HD3	0.453
1	A:95:THR:O	A:95:THR:HG23	0.453
1	A:267:LYS:HD3	A:305:SER:OG	0.451
1	A:234:LYS:N	A:403:THR:HG21	0.451
1	A:102:THR:HG21	A:105:GLU:HA	0.450
1	A:219:PRO:HB3	A:243:LEU:HD21	0.450

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:282:LEU:HD21	A:337:VAL:CG1	0.450
1	A:235:SER:OG	A:245:THR:HG22	0.449
1	A:94:HIS:CD2	A:259:LYS:O	0.445
1	A:353:LYS:HB3	A:375:LYS:HB2	0.445
1	A:341:SER:HB3	A:360:ILE:HA	0.444
1	A:420:VAL:HG21	A:428:LEU:HD22	0.444
1	A:422:SER:HB2	A:434:ALA:O	0.444
1	A:212:THR:CG2	A:214:SER:H	0.443
1	A:215:LEU:HA	A:216:PRO:HA	0.441
1	A:273:GLY:HA2	A:346:PHE:HA	0.440
1	A:275:VAL:HG22	A:344:LEU:HD23	0.438
1	A:233:PRO:CA	A:403:THR:HG21	0.437
1	A:376:LEU:HD13	A:378:PHE:CE1	0.435
1	A:362:HIS:CD2	A:362:HIS:H	0.427
1	A:41:ALA:HB3	A:257:LYS:HD3	0.421
1	A:189:PRO:HG3	A:206:PRO:HB3	0.418
1	A:310:TYR:CD2	A:315:LEU:HD13	0.418
1	A:57:GLU:HG3	A:426:ALA:CB	0.416
1	A:3:GLU:H	A:3:GLU:HG3	0.416
1	A:195:SER:HB3	A:197:TYR:CD1	0.413
1	A:79:LEU:HD13	A:315:LEU:HD11	0.411
1	A:169:THR:HG21	A:174:LYS:N	0.411
1	A:419:MET:HB3	A:419:MET:HE2	0.411

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	A:30:THR:HG22	A:266:LEU:CD2	0.410
1	A:250:MET:H	A:250:MET:HG2	0.409
1	A:187:GLU:HA	A:188:PRO:HD3	0.408
1	A:175:THR:HG23	A:190:LYS:NZ	0.405
1	A:131:SER:H	A:135:THR:HG23	0.403
1	A:357:LEU:H	A:370:LYS:HG3	0.401
1	A:69:THR:CG2	A:71:THR:O	0.400

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.

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	Residue 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

Model ID	Chain	Residue ID	Residue type
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
1	A	169	THR
1	A	211	ARG
1	A	212	THR
1	A	213	PRO
1	A	217	THR
1	A	221	ARG

Model ID	Chain	Residue ID	Residue type
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
1	A	327	ASN
1	A	328	ILE
1	A	339	VAL
1	A	356	SER
1	A	361	THR
1	A	370	LYS

Model ID	Chain	Residue ID	Residue type
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

Crosslinking-MS

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

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