



Full wwPDB EM Validation Report ⓘ

Feb 27, 2025 – 03:06 pm GMT

PDB ID : 8BGS
EMDB ID : EMD-16035
Title : Tau Paired Helical Filament from Extracellular Vesicles from Alzheimer's disease brain
Authors : Behr, T.S.; Ryskeldi-Falcon, B.
Deposited on : 2022-10-28
Resolution : 3.16 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

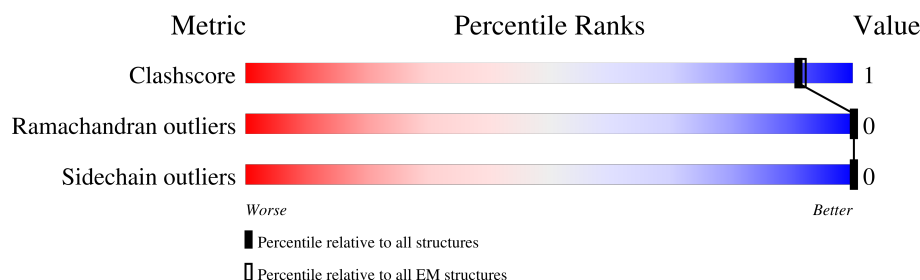
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	441	16% . 83%
1	B	441	16% . 83%
1	C	441	16% . 83%
1	D	441	16% . 83%
1	E	441	16% . 83%
1	F	441	16% . 83%
1	r	441	17% 83%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4018 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Microtubule-associated protein tau.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	r	75	Total	C	N	O	S	0	0
			574	360	106	107	1		
1	A	75	Total	C	N	O	S	0	0
			574	360	106	107	1		
1	B	75	Total	C	N	O	S	0	0
			574	360	106	107	1		
1	C	75	Total	C	N	O	S	0	0
			574	360	106	107	1		
1	D	75	Total	C	N	O	S	0	0
			574	360	106	107	1		
1	E	75	Total	C	N	O	S	0	0
			574	360	106	107	1		
1	F	75	Total	C	N	O	S	0	0
			574	360	106	107	1		

- Molecule 1: Microtubule-associated protein tau

- Molecule 1: Microtubule-associated protein tau





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=179.439°, rise=2.354 Å, axial sym=C1	Depositor
Number of segments used	18041	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38.7	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/583	0.79	0/780
1	B	0.42	0/583	0.79	0/780
1	C	0.42	0/583	0.79	0/780
1	D	0.42	0/583	0.79	0/780
1	E	0.42	0/583	0.79	0/780
1	F	0.42	0/583	0.79	0/780
1	r	0.42	0/583	0.79	0/780
All	All	0.42	0/4081	0.79	0/5460

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	r	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	B	321	LYS	Peptide
1	C	321	LYS	Peptide
1	D	321	LYS	Peptide
1	E	321	LYS	Peptide
1	F	321	LYS	Peptide
1	r	321	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	574	0	597	2	0
1	B	574	0	597	1	0
1	C	574	0	597	3	0
1	D	574	0	597	2	0
1	E	574	0	597	2	0
1	F	574	0	597	2	0
1	r	574	0	597	0	0
All	All	4018	0	4179	9	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (9) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:HIS:CD2	1:B:364:PRO:HD3	2.47	0.49
1:F:362:HIS:CD2	1:F:364:PRO:HD3	2.47	0.49
1:A:362:HIS:CD2	1:A:364:PRO:HD3	2.47	0.49
1:C:362:HIS:CD2	1:C:364:PRO:HD3	2.47	0.49
1:E:362:HIS:CD2	1:E:364:PRO:HD3	2.47	0.49
1:D:362:HIS:CD2	1:D:364:PRO:HD3	2.47	0.49
1:E:364:PRO:HG2	1:F:364:PRO:HB3	2.01	0.42
1:A:364:PRO:HG2	1:C:364:PRO:HB3	2.01	0.42
1:C:364:PRO:HG2	1:D:364:PRO:HB3	2.01	0.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	73/441 (17%)	68 (93%)	5 (7%)	0	100	100
1	B	73/441 (17%)	68 (93%)	5 (7%)	0	100	100
1	C	73/441 (17%)	68 (93%)	5 (7%)	0	100	100
1	D	73/441 (17%)	68 (93%)	5 (7%)	0	100	100
1	E	73/441 (17%)	68 (93%)	5 (7%)	0	100	100
1	F	73/441 (17%)	68 (93%)	5 (7%)	0	100	100
1	r	73/441 (17%)	68 (93%)	5 (7%)	0	100	100
All	All	511/3087 (17%)	476 (93%)	35 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	66/358 (18%)	66 (100%)	0	100	100
1	B	66/358 (18%)	66 (100%)	0	100	100
1	C	66/358 (18%)	66 (100%)	0	100	100
1	D	66/358 (18%)	66 (100%)	0	100	100
1	E	66/358 (18%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	66/358 (18%)	66 (100%)	0	100	100
1	r	66/358 (18%)	66 (100%)	0	100	100
All	All	462/2506 (18%)	462 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	r	330	HIS
1	r	362	HIS
1	A	330	HIS
1	A	362	HIS
1	B	330	HIS
1	B	362	HIS
1	C	330	HIS
1	C	362	HIS
1	D	330	HIS
1	D	362	HIS
1	E	330	HIS
1	E	362	HIS
1	F	330	HIS
1	F	362	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.