Full wwPDB EM Validation Report ⓘ

Oct 26, 2026 – 04:13 PM JST

PDB ID	:	9XHU / pdb_00009xhu
EMDB ID	:	EMD-66886
Title	:	The cryo-EM structure of ThS bound Tau PHF fibril
Authors	:	Zhao, Q.Y.; Cao, T.Y.; Liu, C.; Li, D.
Deposited on	:	2025-11-02
Resolution	:	3.40 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:

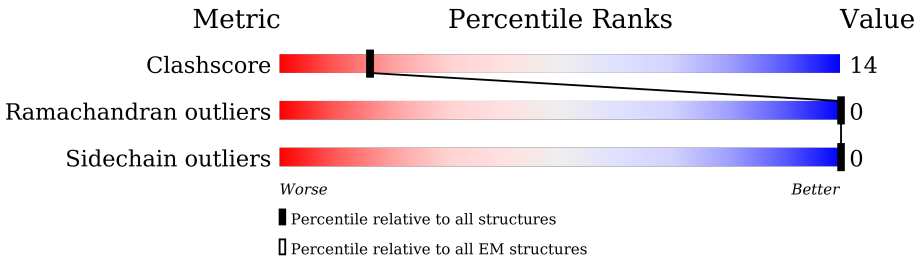
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

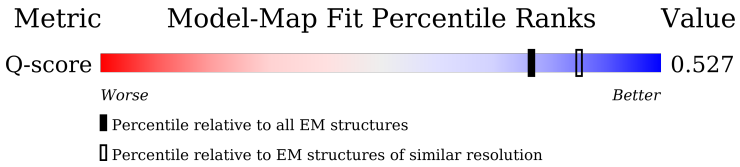
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.





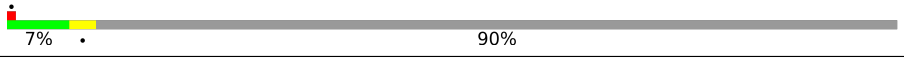
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	758	7% · 90%
1	B	758	7% · 90%
1	C	758	7% · 90%
1	D	758	7% · 90%

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Mol	Chain	Length	Quality of chain
1	E	758	
1	F	758	

2 Entry composition

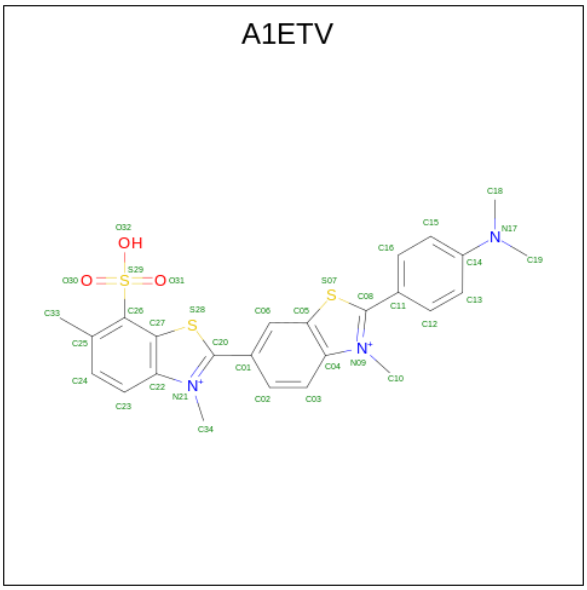
There are 2 unique types of molecules in this entry. The entry contains 3510 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isoform PNS-tau of Microtubule-associated protein tau.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	74	Total	C	N	O	S	0	0
			568	357	105	105	1		
1	B	74	Total	C	N	O	S	0	0
			568	357	105	105	1		
1	C	74	Total	C	N	O	S	0	0
			568	357	105	105	1		
1	D	74	Total	C	N	O	S	0	0
			568	357	105	105	1		
1	E	74	Total	C	N	O	S	0	0
			568	357	105	105	1		
1	F	74	Total	C	N	O	S	0	0
			568	357	105	105	1		

- Molecule 2 is 2-[2-[4-(dimethylamino)phenyl]-3-methyl-1,3-benzothiazol-3-ium-6-yl]-3,6-dimethyl-1,3-benzothiazol-3-ium-7-sulfonic acid (CCD ID: A1ETV) (formula: $C_{25}H_{25}N_3O_3S_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			34	25	3	3	3	
2	A	1	Total	C	N	O	S	0
			34	25	3	3	3	
2	E	1	Total	C	N	O	S	0
			34	25	3	3	3	

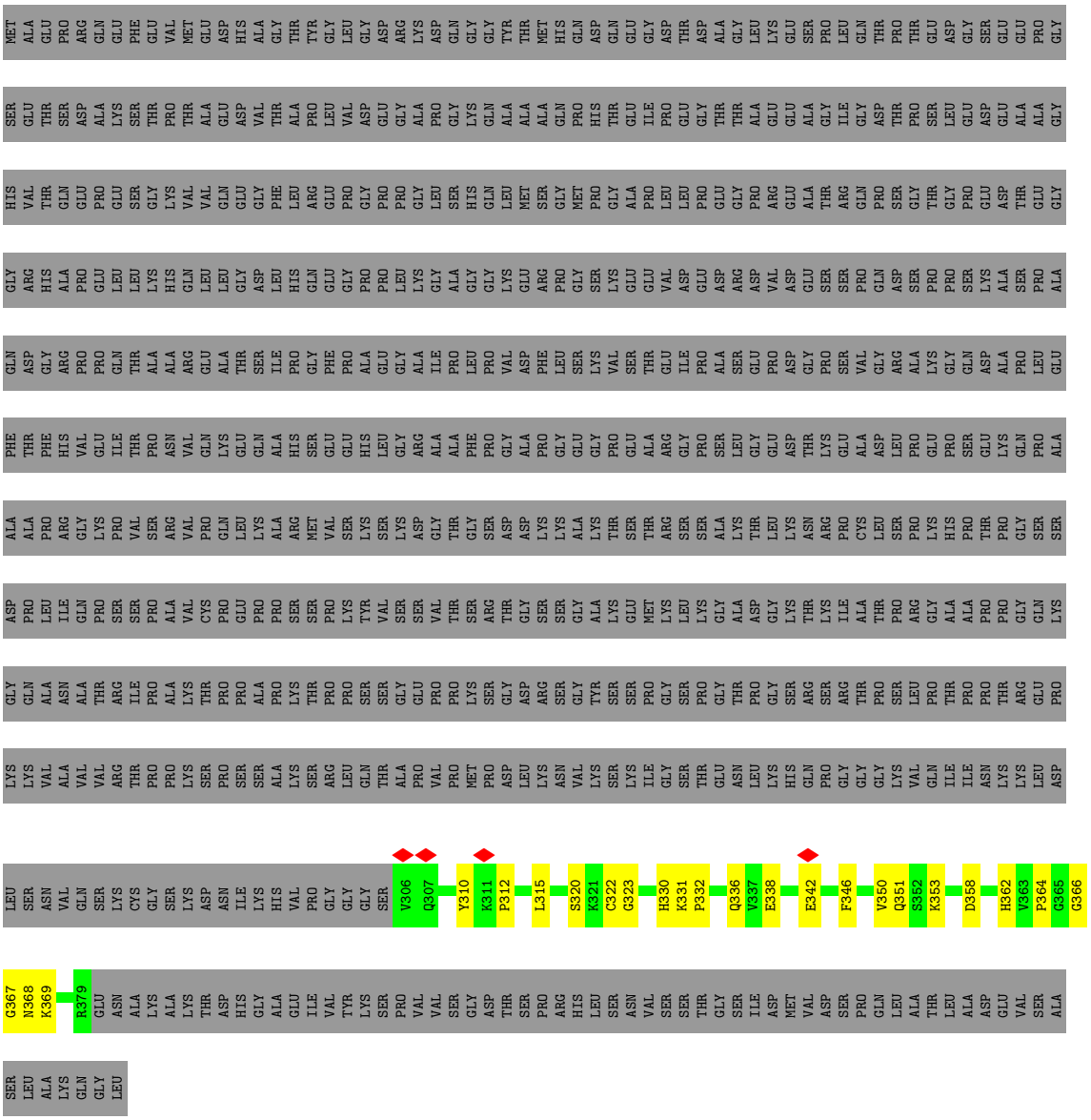
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Isoform PNS-tau of Microtubule-associated protein tau

Chain A:

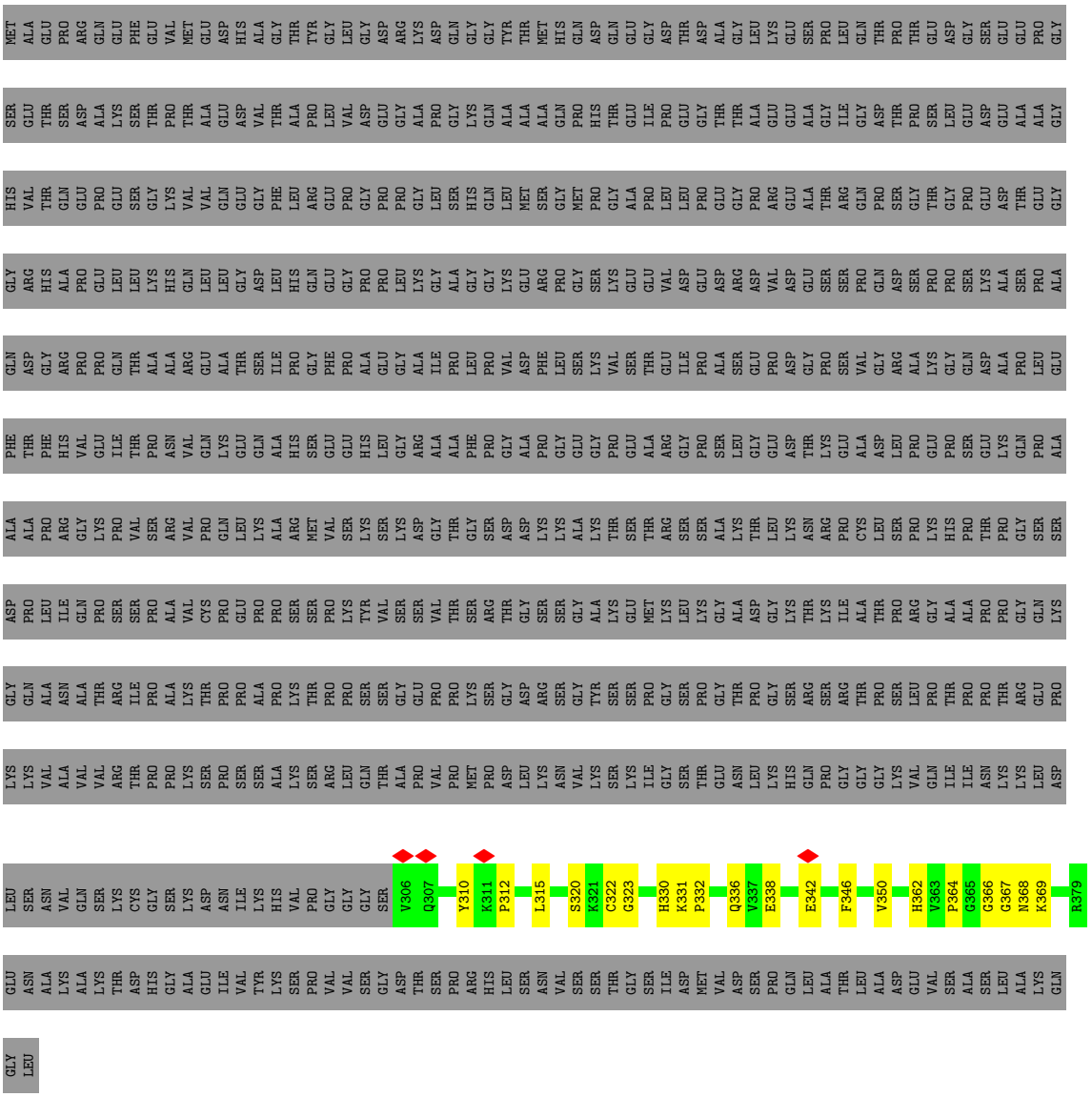




• Molecule 1: Isoform PNS-tau of Microtubule-associated protein tau

Chain B:

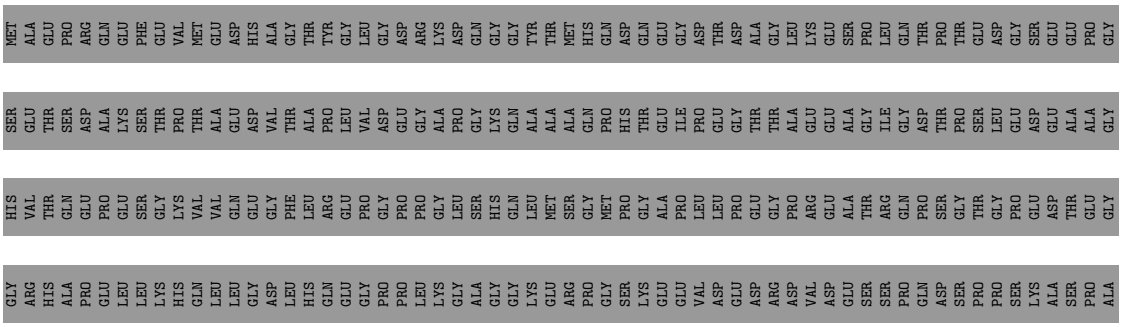


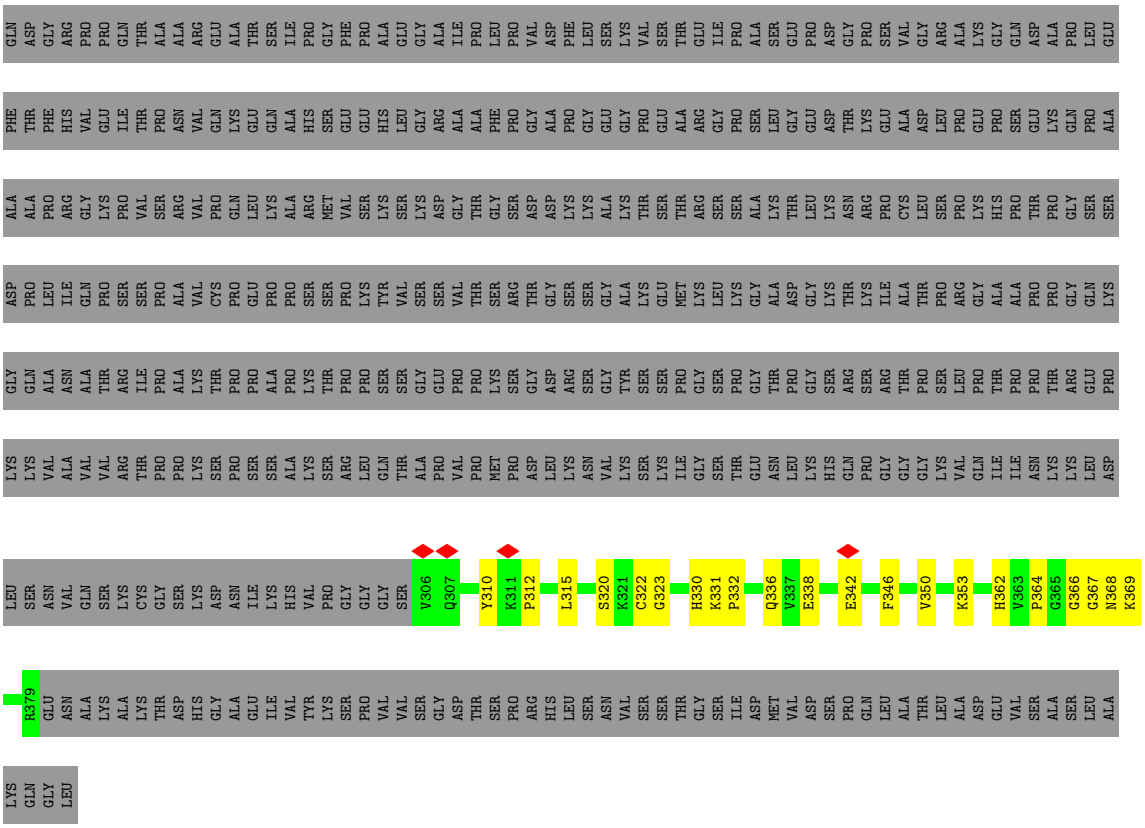


• Molecule 1: Isoform PNS-tau of Microtubule-associated protein tau

Chain C:

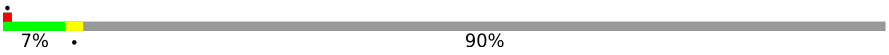


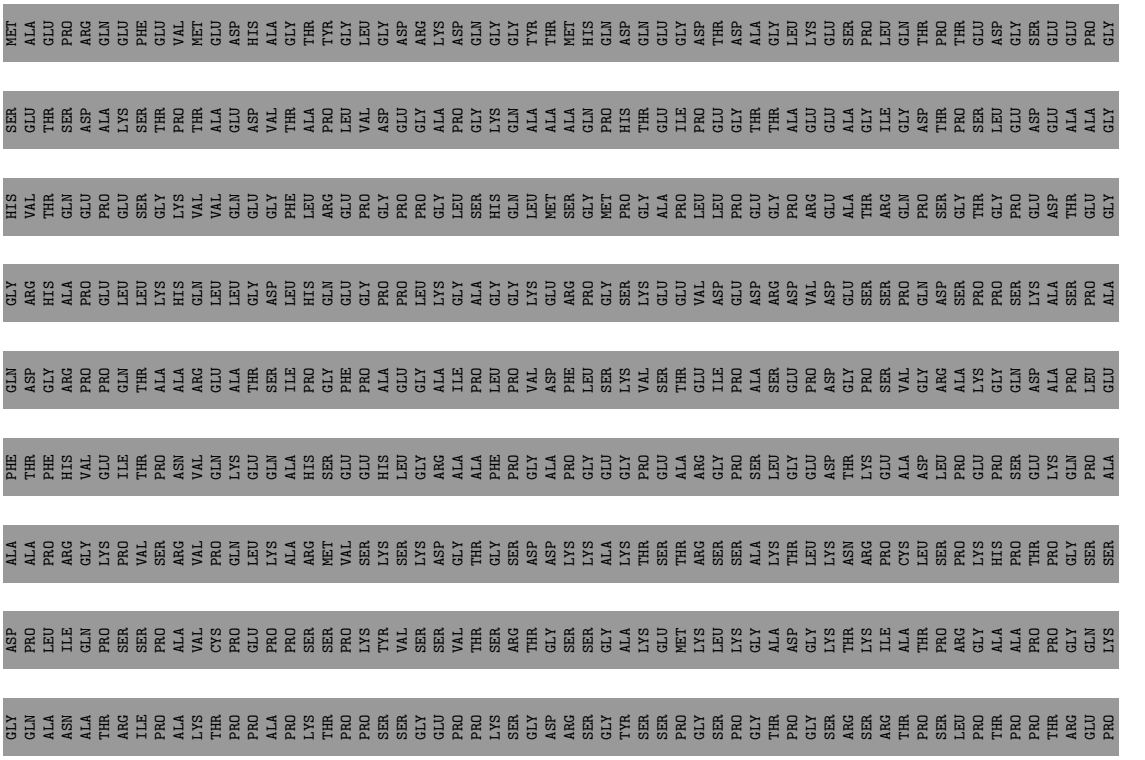


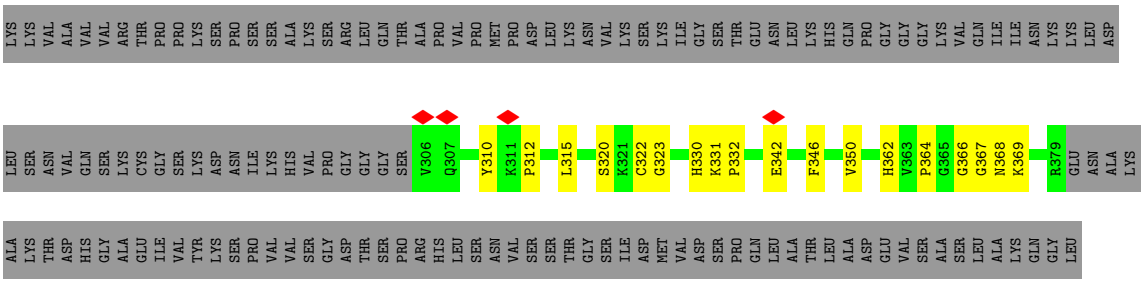


• Molecule 1: Isoform PNS-tau of Microtubule-associated protein tau

Chain D:



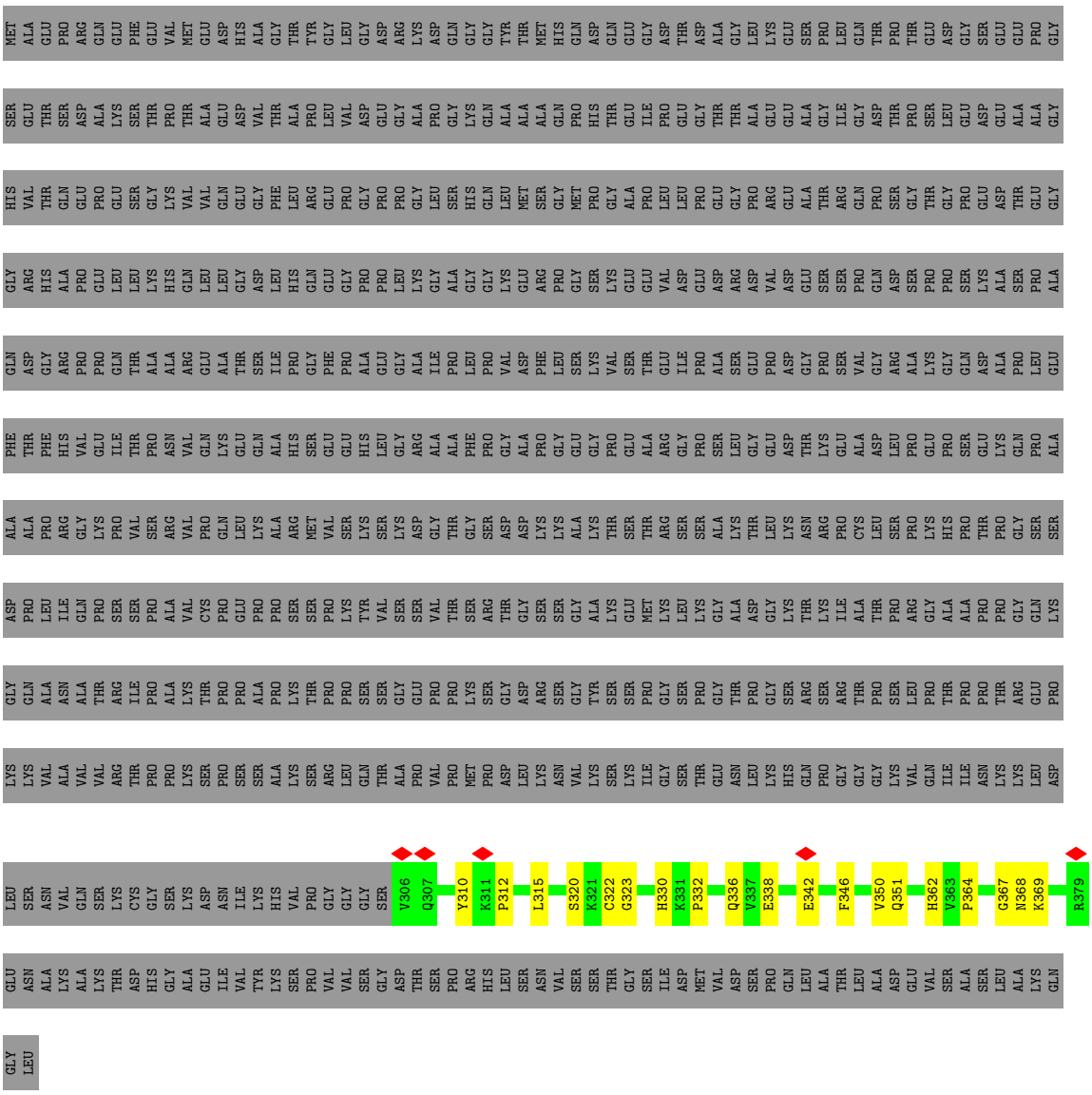




• Molecule 1: Isoform PNS-tau of Microtubule-associated protein tau

Chain E:

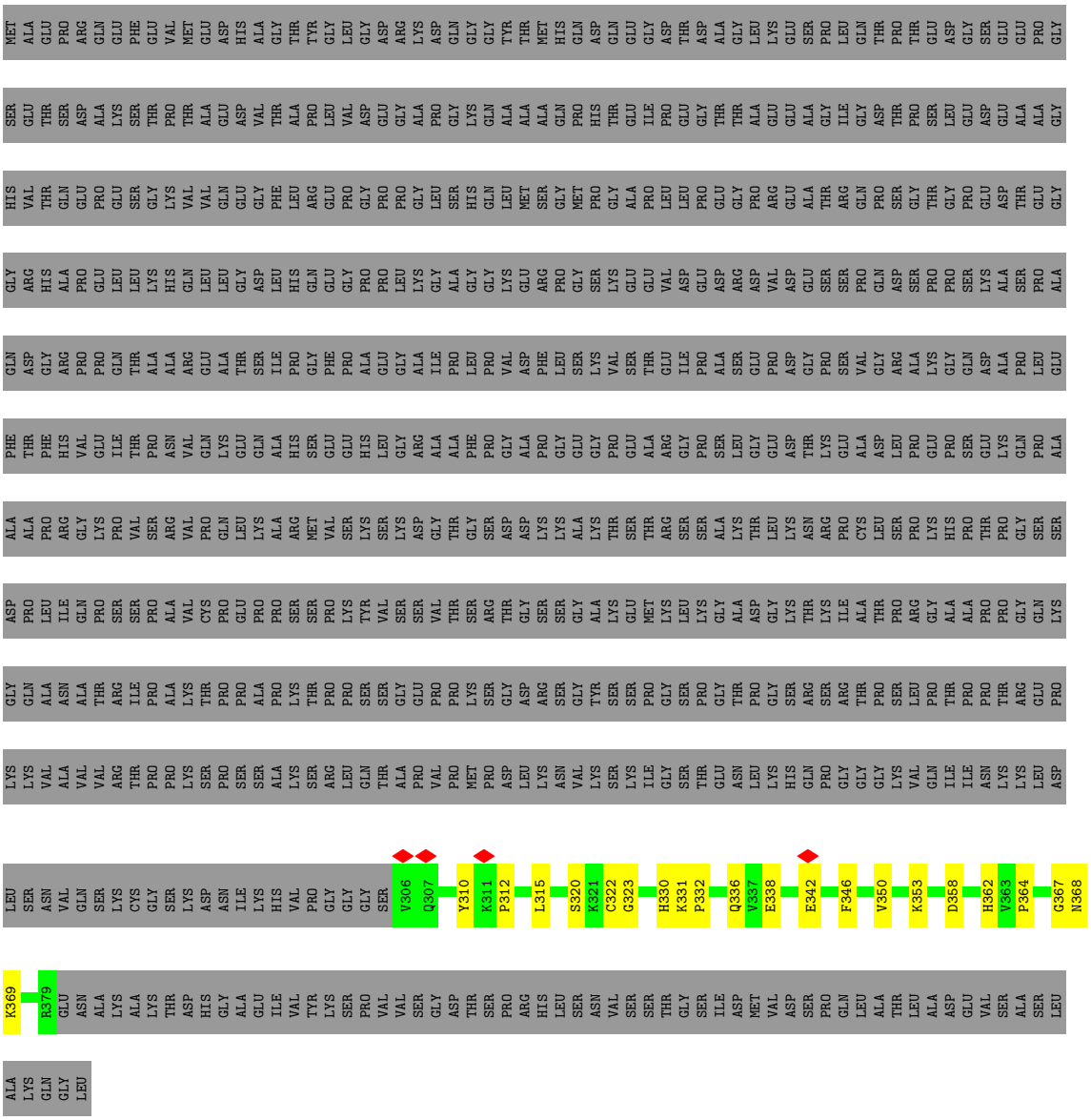




• Molecule 1: Isoform PNS-tau of Microtubule-associated protein tau

Chain F:




MET ALA GLU PRO ARG GLN GLU PHE GLU VAL MET GLU ASP HIS ALA GLY THR TYR GLY LEU GLY ASP ARG LYS ASP GLN GLY GLY TYR THR MET HIS GLN ASP GLN GLU GLY ASP THR ASP ALA GLY LEU LYS GLU SER PRO LEU GLN THR PRO THR GLU ASP GLY SER GLU GLU PRO ALA GLY
SER GLU THR SER ASP ALA LYS SER THR PRO THR ALA GLU ASP VAL THR ALA PRO LEU VAL ASP GLU GLY ALA PRO GLY LYS GLN ALA ALA ALA ALA GLN PRO HIS THR GLU ILE PRO GLU GLY THR THR ALA GLU GLU ALA GLY ILE GLY ASP THR PRO SER LEU GLU ASP GLU ALA GLY
HIS VAL THR GLN GLU PRO GLU SER GLY LYS VAL VAL GLN GLU GLY PHE LEU ARG GLU PRO GLY PRO PRO GLY LEU SER HIS GLN LEU MET SER GLY MET PRO GLY ALA PRO LEU LEU PRO GLU GLY GLY PRO GLU GLY ARG GLN PRO SER GLY THR GLY PRO GLU GLU ASP THR GLU GLY
GLY ARG HIS ALA PRO GLU LEU LEU LYS HIS GLN LEU LEU LEU GLY ASP LEU HIS GLN GLU GLY PRO PRO LEU LYS GLY ALA GLY GLY LYS SER LYS GLU GLU VAL ASP GLU ASP ARG ASP VAL ASP GLU SER SER PRO SER PRO PRO SER LYS ALA SER PRO ALA
GLN ASP GLY ARG PRO PRO GLN THR ALA ALA ARG GLU ALA THR SER ILE PRO GLY PHE PRO ALA GLU GLY ALA ILE PRO LEU PRO VAL ASP PHE LEU SER LYS SER GLU THR GLU ILE PRO ALA SER GLU PRO ASP GLY PRO SER VAL GLY ARG ALA LYS GLY GLN ASP ALA PRO LEU GLU
PHE THR PHE HIS VAL GLU ILE THR PRO ASN VAL GLN LYS GLU GLU GLN ALA HIS SER GLU GLU HIS LEU GLY ARG ALA ALA PHE PRO GLY ALA PRO GLY GLU GLY GLU ASP THR LYS GLU ALA ASP LEU PRO GLU GLY GLN PRO ALA
ALA ALA PRO ARG GLY LYS PRO VAL SER ARG VAL PRO GLN LEU LYS ALA ARG MET VAL SER LYS SER LYS ASP GLY THR GLY SER ASP ASP LYS LYS ALA LYS THR SER THR ARG SER SER ALA LYS THR LEU LYS ASN ARG PRO CYS LEU SER PRO LYS HIS PRO THR PRO GLY SER
ASP PRO LEU ILE GLN PRO SER SER PRO ALA VAL CYS PRO GLU PRO PRO SER SER PRO LYS TYR VAL SER SER VAL THR SER ARG THR GLY SER ALA LYS GLU MET LYS LEU LYS GLY ALA ASP GLY LYS THR LEU LYS ILE LEU PRO THR ARG ILE PRO ALA GLY GLY GLN LYS
GLY GLN ALA ASN ALA THR ARG ILE PRO ALA LYS THR PRO PRO PRO ALA PRO LYS THR PRO PRO SER SER GLY GLU PRO PRO VAL PRO PRO LYS SER ASP ARG SER GLY TYR SER SER PRO GLY SER PRO GLY THR PRO GLY SER ARG SER ARG THR PRO SER LEU PRO THR PRO PRO THR ARG GLU PRO
LYS LYS VAL ALA VAL VAL ARG THR PRO PRO LYS SER PRO SER SER ALA LYS SER ARG LEU GLN LEU THR ALA PRO VAL PRO MET PRO ASP LEU LYS ASN VAL LYS SER LYS ILE GLY SER THR GLU ASN LEU LYS HIS GLN PRO GLY GLY GLY LYS VAL GLN ILE ILE ASN LYS LYS LEU ASP
V306 Q307 Y310 K311 P312 L315 S320 K321 C322 G323 H330 K331 P332 Q336 V337 E338 E342 F346 V350 K353 D358 H362 V363 P364 G367 N368
LEU SER ASN VAL GLN SER LYS CYS GLY SER LYS ASP ASN ILE LYS HIS VAL PRO GLY GLY GLY SER
K369 R379
GLU ASN ALA LYS ALA LYS THR ASP HIS GLY ALA GLU ILE VAL TYR LYS SER PRO VAL VAL SER GLY ASP THR SER PRO ARG HIS LEU SER ASN VAL SER SER THR GLY SER ILE ASP MET VAL ASP SER PRO GLN LEU ALA THR LEU ALA ASP GLU VAL SER ALA SER LEU
ALA LYS GLN GLY LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=179.426°, rise=2.396 Å, axial sym=C1	Depositor
Number of segments used	14487	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0041	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1ETV

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	0.30	0/577	0.41	0/772
1	B	0.30	0/577	0.41	0/772
1	C	0.30	0/577	0.41	0/772
1	D	0.30	0/577	0.41	0/772
1	E	0.30	0/577	0.41	0/772
1	F	0.30	0/577	0.41	0/772
All	All	0.30	0/3462	0.41	0/4632

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	568	0	592	37	0
1	B	568	0	592	26	0
1	C	568	0	592	21	0
1	D	568	0	592	17	0
1	E	568	0	592	21	0
1	F	568	0	592	20	0
2	A	68	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	34	0	0	2	0
All	All	3510	0	3552	101	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 14.

All (101) 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:315:LEU:HB2	1:D:315:LEU:HD23	1.39	1.04
1:B:315:LEU:HD23	1:F:315:LEU:HB2	1.39	1.03
1:A:315:LEU:HD23	1:E:315:LEU:HB2	1.40	1.00
1:A:315:LEU:HB2	1:C:315:LEU:HD23	1.39	1.00
1:A:315:LEU:HB2	1:C:315:LEU:CD2	1.96	0.96
1:A:315:LEU:CD2	1:E:315:LEU:HB2	1.97	0.95
1:B:315:LEU:HB2	1:D:315:LEU:CD2	1.96	0.94
1:B:315:LEU:CD2	1:F:315:LEU:HB2	1.96	0.94
1:A:369:LYS:HG2	2:A:501:A1ETV:C18	2.06	0.86
1:B:315:LEU:HD12	1:D:315:LEU:HD21	1.67	0.76
1:B:315:LEU:HD21	1:F:315:LEU:HD12	1.67	0.76
1:A:315:LEU:HD12	1:C:315:LEU:HD21	1.68	0.74
1:A:315:LEU:HD21	1:E:315:LEU:HD12	1.68	0.74
1:A:369:LYS:HE3	2:A:501:A1ETV:C15	2.19	0.72
1:A:353:LYS:HB2	2:A:502:A1ETV:O31	1.92	0.70
1:E:362:HIS:CD2	1:E:364:PRO:HD3	2.33	0.64
1:A:362:HIS:CD2	1:A:364:PRO:HD3	2.33	0.63
1:C:362:HIS:CD2	1:C:364:PRO:HD3	2.33	0.63
1:B:367:GLY:O	1:D:367:GLY:HA2	1.98	0.63
1:A:367:GLY:O	1:C:367:GLY:HA2	1.99	0.63
1:B:367:GLY:HA2	1:F:367:GLY:O	1.99	0.63
2:A:501:A1ETV:O31	1:C:353:LYS:HB2	1.99	0.63
1:F:362:HIS:CD2	1:F:364:PRO:HD3	2.33	0.63
1:A:367:GLY:HA2	1:E:367:GLY:O	1.99	0.62
1:D:362:HIS:CD2	1:D:364:PRO:HD3	2.33	0.62
1:B:362:HIS:CD2	1:B:364:PRO:HD3	2.33	0.62
1:E:336:GLN:HE22	1:F:331:LYS:HB3	1.63	0.62
1:F:346:PHE:HB3	1:F:350:VAL:HG21	1.83	0.60
1:D:346:PHE:HB3	1:D:350:VAL:HG21	1.83	0.60
1:B:346:PHE:HB3	1:B:350:VAL:HG21	1.83	0.60
1:A:346:PHE:HB3	1:A:350:VAL:HG21	1.83	0.60
1:E:346:PHE:HB3	1:E:350:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:PHE:HB3	1:C:350:VAL:HG21	1.83	0.59
1:A:331:LYS:HB3	1:F:336:GLN:HE22	1.68	0.59
1:A:336:GLN:HE22	1:B:331:LYS:HB3	1.68	0.57
1:A:362:HIS:HE1	2:A:502:A1ETV:C12	2.17	0.57
1:A:369:LYS:NZ	2:A:501:A1ETV:C16	2.67	0.57
1:B:336:GLN:HE22	1:C:331:LYS:HB3	1.70	0.57
1:C:336:GLN:HE22	1:D:331:LYS:HB3	1.69	0.56
1:A:351:GLN:OE1	2:A:502:A1ETV:C24	2.54	0.56
2:A:502:A1ETV:C18	1:E:369:LYS:HG2	2.36	0.55
1:E:351:GLN:OE1	2:E:501:A1ETV:C24	2.55	0.55
1:A:369:LYS:CE	2:A:501:A1ETV:C15	2.86	0.53
1:B:320:SER:OG	1:D:366:GLY:HA3	2.07	0.53
1:A:366:GLY:HA3	1:E:320:SER:OG	2.09	0.53
1:A:342:GLU:HB2	1:C:342:GLU:O	2.08	0.53
1:B:366:GLY:HA3	1:F:320:SER:OG	2.08	0.53
1:B:342:GLU:HB2	1:D:342:GLU:O	2.08	0.53
1:A:320:SER:OG	1:C:366:GLY:HA3	2.09	0.52
1:E:338:GLU:OE1	1:F:331:LYS:NZ	2.43	0.52
1:C:330:HIS:CD2	1:C:332:PRO:HD3	2.45	0.52
1:D:330:HIS:CD2	1:D:332:PRO:HD3	2.45	0.52
1:A:330:HIS:CD2	1:A:332:PRO:HD3	2.45	0.51
1:F:330:HIS:CD2	1:F:332:PRO:HD3	2.45	0.51
1:B:330:HIS:CD2	1:B:332:PRO:HD3	2.45	0.51
1:A:369:LYS:H	2:A:501:A1ETV:C18	2.24	0.51
1:E:330:HIS:CD2	1:E:332:PRO:HD3	2.45	0.51
1:A:342:GLU:O	1:E:342:GLU:HB2	2.10	0.51
1:B:342:GLU:O	1:F:342:GLU:HB2	2.10	0.50
1:C:338:GLU:OE1	1:D:331:LYS:NZ	2.45	0.50
1:B:338:GLU:OE1	1:C:331:LYS:NZ	2.44	0.50
1:A:331:LYS:NZ	1:F:338:GLU:OE1	2.44	0.50
1:F:322:CYS:SG	1:F:323:GLY:N	2.85	0.50
1:C:322:CYS:SG	1:C:323:GLY:N	2.85	0.50
1:B:322:CYS:SG	1:B:323:GLY:N	2.85	0.50
1:A:338:GLU:OE1	1:B:331:LYS:NZ	2.46	0.49
1:A:322:CYS:SG	1:A:323:GLY:N	2.85	0.49
1:D:322:CYS:SG	1:D:323:GLY:N	2.85	0.49
1:E:322:CYS:SG	1:E:323:GLY:N	2.85	0.49
1:B:310:TYR:CD1	1:B:312:PRO:HD3	2.49	0.48
1:A:310:TYR:CD1	1:A:312:PRO:HD3	2.49	0.48
1:D:310:TYR:CD1	1:D:312:PRO:HD3	2.49	0.48
1:F:310:TYR:CD1	1:F:312:PRO:HD3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:TYR:CD1	1:C:312:PRO:HD3	2.49	0.47
1:E:310:TYR:CD1	1:E:312:PRO:HD3	2.49	0.47
1:E:362:HIS:HE1	2:E:501:A1ETV:C12	2.28	0.47
1:A:320:SER:HB3	1:A:368:ASN:HD21	1.81	0.46
1:C:320:SER:HB3	1:C:368:ASN:HD21	1.81	0.46
1:E:320:SER:HB3	1:E:368:ASN:HD21	1.81	0.46
1:F:320:SER:HB3	1:F:368:ASN:HD21	1.81	0.46
1:B:320:SER:HB3	1:B:368:ASN:HD21	1.81	0.46
1:D:320:SER:HB3	1:D:368:ASN:HD21	1.81	0.46
1:F:353:LYS:NZ	1:F:358:ASP:OD2	2.50	0.45
1:B:312:PRO:HA	1:D:312:PRO:HD2	2.00	0.44
1:B:312:PRO:HD2	1:F:312:PRO:HA	2.00	0.44
1:A:312:PRO:HA	1:C:312:PRO:HD2	2.00	0.43
2:A:502:A1ETV:C15	1:E:369:LYS:HE3	2.48	0.43
1:A:312:PRO:HD2	1:E:312:PRO:HA	2.00	0.43
1:E:362:HIS:HD2	1:E:364:PRO:HD3	1.81	0.43
1:A:362:HIS:HD2	1:A:364:PRO:HD3	1.81	0.42
1:B:369:LYS:HD2	1:D:369:LYS:HE2	2.01	0.42
2:A:501:A1ETV:O31	2:A:502:A1ETV:O32	2.37	0.42
1:A:353:LYS:NZ	1:A:358:ASP:OD2	2.50	0.41
1:C:362:HIS:HD2	1:C:364:PRO:HD3	1.81	0.41
1:B:369:LYS:HE2	1:F:369:LYS:HD2	2.02	0.41
1:C:336:GLN:HE22	1:D:331:LYS:HD3	1.86	0.41
1:A:362:HIS:CE1	2:A:502:A1ETV:C12	3.02	0.41
1:A:369:LYS:HD2	1:C:369:LYS:HE2	2.02	0.41
1:A:369:LYS:HE2	1:E:369:LYS:HD2	2.02	0.41
1:F:362:HIS:HD2	1:F:364:PRO:HD3	1.81	0.41
2:A:501:A1ETV:S29	2:A:502:A1ETV:O32	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	72/758 (10%)	63 (88%)	9 (12%)	0	100	100
1	B	72/758 (10%)	63 (88%)	9 (12%)	0	100	100
1	C	72/758 (10%)	63 (88%)	9 (12%)	0	100	100
1	D	72/758 (10%)	63 (88%)	9 (12%)	0	100	100
1	E	72/758 (10%)	63 (88%)	9 (12%)	0	100	100
1	F	72/758 (10%)	63 (88%)	9 (12%)	0	100	100
All	All	432/4548 (10%)	378 (88%)	54 (12%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	65/616 (11%)	65 (100%)	0	100	100
1	B	65/616 (11%)	65 (100%)	0	100	100
1	C	65/616 (11%)	65 (100%)	0	100	100
1	D	65/616 (11%)	65 (100%)	0	100	100
1	E	65/616 (11%)	65 (100%)	0	100	100
1	F	65/616 (11%)	65 (100%)	0	100	100
All	All	390/3696 (11%)	390 (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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	A	362	HIS
1	B	336	GLN
1	B	362	HIS
1	C	330	HIS

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Mol	Chain	Res	Type
1	C	336	GLN
1	C	362	HIS
1	C	368	ASN
1	D	330	HIS
1	D	362	HIS
1	D	368	ASN
1	E	336	GLN
1	E	362	HIS
1	F	329	HIS
1	F	336	GLN
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

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	A1ETV	A	502	-	35,38,38	1.43	5 (14%)	52,59,59	2.46	19 (36%)
2	A1ETV	E	501	-	35,38,38	1.43	5 (14%)	52,59,59	2.47	19 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	A1ETV	A	501	-	35,38,38	1.43	5 (14%)	52,59,59	2.47	19 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1ETV	A	502	-	-	10/18/18/18	0/5/5/5
2	A1ETV	E	501	-	-	10/18/18/18	0/5/5/5
2	A1ETV	A	501	-	-	10/18/18/18	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	A1ETV	C14-N17	3.59	1.45	1.37
2	A	501	A1ETV	C14-N17	3.57	1.45	1.37
2	A	501	A1ETV	C11-C08	-3.56	1.40	1.47
2	A	502	A1ETV	C14-N17	3.56	1.45	1.37
2	E	501	A1ETV	C11-C08	-3.55	1.40	1.47
2	A	502	A1ETV	C11-C08	-3.54	1.40	1.47
2	E	501	A1ETV	C01-C20	-3.35	1.40	1.47
2	A	501	A1ETV	C01-C20	-3.34	1.40	1.47
2	A	502	A1ETV	C01-C20	-3.33	1.40	1.47
2	A	501	A1ETV	C04-N09	-2.38	1.36	1.40
2	E	501	A1ETV	C04-N09	-2.33	1.36	1.40
2	A	502	A1ETV	C04-N09	-2.31	1.36	1.40
2	A	501	A1ETV	C22-N21	-2.21	1.36	1.40
2	E	501	A1ETV	C22-N21	-2.20	1.36	1.40
2	A	502	A1ETV	C22-N21	-2.19	1.36	1.40

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	A1ETV	C05-S07-C08	6.62	95.51	89.80
2	A	501	A1ETV	C05-S07-C08	6.60	95.49	89.80
2	A	502	A1ETV	C05-S07-C08	6.57	95.46	89.80
2	A	501	A1ETV	C04-C05-S07	-5.84	103.94	110.19
2	E	501	A1ETV	C04-C05-S07	-5.82	103.95	110.19
2	A	502	A1ETV	C04-C05-S07	-5.80	103.98	110.19
2	E	501	A1ETV	C22-C27-S28	-5.28	105.39	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	A1ETV	C22-C27-S28	-5.27	105.41	110.06
2	A	502	A1ETV	C22-C27-S28	-5.27	105.41	110.06
2	E	501	A1ETV	C27-C26-S29	-5.26	117.70	122.52
2	A	502	A1ETV	C27-C26-S29	-5.24	117.72	122.52
2	A	501	A1ETV	C27-C26-S29	-5.23	117.73	122.52
2	A	501	A1ETV	C05-C04-N09	4.37	117.63	112.05
2	E	501	A1ETV	C05-C04-N09	4.36	117.61	112.05
2	A	502	A1ETV	C05-C04-N09	4.34	117.60	112.05
2	A	501	A1ETV	C02-C01-C20	-4.24	114.37	120.58
2	A	502	A1ETV	C02-C01-C20	-4.23	114.38	120.58
2	E	501	A1ETV	C02-C01-C20	-4.22	114.40	120.58
2	E	501	A1ETV	C06-C01-C20	4.19	126.68	120.57
2	A	501	A1ETV	C06-C01-C20	4.17	126.65	120.57
2	A	502	A1ETV	C06-C01-C20	4.12	126.59	120.57
2	E	501	A1ETV	C06-C05-S07	3.72	135.74	126.07
2	A	501	A1ETV	C06-C05-S07	3.71	135.73	126.07
2	A	502	A1ETV	C06-C05-S07	3.70	135.70	126.07
2	A	502	A1ETV	C27-C22-N21	3.49	116.49	112.03
2	A	501	A1ETV	C27-C22-N21	3.48	116.48	112.03
2	A	501	A1ETV	C03-C04-N09	-3.48	122.16	129.25
2	E	501	A1ETV	C03-C04-N09	-3.48	122.16	129.25
2	A	502	A1ETV	C03-C04-N09	-3.47	122.17	129.25
2	E	501	A1ETV	C27-C22-N21	3.46	116.44	112.03
2	E	501	A1ETV	C24-C25-C26	3.39	119.55	116.69
2	A	501	A1ETV	C24-C25-C26	3.35	119.52	116.69
2	A	502	A1ETV	C24-C25-C26	3.31	119.49	116.69
2	E	501	A1ETV	O31-S29-C26	2.86	113.46	106.38
2	A	501	A1ETV	O31-S29-C26	2.85	113.44	106.38
2	A	502	A1ETV	O31-S29-C26	2.85	113.44	106.38
2	E	501	A1ETV	C11-C08-S07	2.77	125.42	120.93
2	A	501	A1ETV	C11-C08-S07	2.76	125.41	120.93
2	A	502	A1ETV	C11-C08-S07	2.74	125.37	120.93
2	E	501	A1ETV	C34-N21-C22	-2.56	117.83	122.69
2	A	501	A1ETV	C34-N21-C22	-2.53	117.88	122.69
2	A	502	A1ETV	C34-N21-C22	-2.53	117.88	122.69
2	A	502	A1ETV	C23-C22-N21	-2.49	124.18	129.25
2	A	501	A1ETV	C23-C22-N21	-2.48	124.19	129.25
2	E	501	A1ETV	C23-C22-N21	-2.46	124.24	129.25
2	E	501	A1ETV	O30-S29-C26	2.36	112.23	106.38
2	A	501	A1ETV	O30-S29-C26	2.36	112.22	106.38
2	A	502	A1ETV	O30-S29-C26	2.35	112.20	106.38
2	E	501	A1ETV	O31-S29-O30	-2.27	101.05	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	A1ETV	O31-S29-O30	-2.26	101.10	112.86
2	A	502	A1ETV	O31-S29-O30	-2.26	101.12	112.86
2	E	501	A1ETV	C33-C25-C26	-2.26	121.88	125.16
2	A	501	A1ETV	C33-C25-C26	-2.22	121.93	125.16
2	A	501	A1ETV	C04-N09-C08	2.21	116.61	114.17
2	A	502	A1ETV	C33-C25-C26	-2.20	121.95	125.16
2	A	502	A1ETV	C04-N09-C08	2.20	116.60	114.17
2	E	501	A1ETV	C04-N09-C08	2.20	116.59	114.17

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1ETV	C02-C01-C20-N21
2	A	501	A1ETV	C06-C01-C20-N21
2	A	501	A1ETV	C25-C26-S29-O32
2	A	501	A1ETV	C27-C26-S29-O32
2	A	502	A1ETV	C02-C01-C20-N21
2	A	502	A1ETV	C06-C01-C20-N21
2	A	502	A1ETV	C25-C26-S29-O32
2	A	502	A1ETV	C27-C26-S29-O32
2	E	501	A1ETV	C02-C01-C20-N21
2	E	501	A1ETV	C06-C01-C20-N21
2	E	501	A1ETV	C25-C26-S29-O32
2	E	501	A1ETV	C27-C26-S29-O32
2	E	501	A1ETV	C15-C14-N17-C19
2	A	501	A1ETV	C15-C14-N17-C19
2	A	502	A1ETV	C15-C14-N17-C19
2	A	501	A1ETV	C02-C01-C20-S28
2	A	501	A1ETV	C06-C01-C20-S28
2	A	502	A1ETV	C02-C01-C20-S28
2	A	502	A1ETV	C06-C01-C20-S28
2	E	501	A1ETV	C02-C01-C20-S28
2	E	501	A1ETV	C06-C01-C20-S28
2	A	501	A1ETV	C13-C14-N17-C18
2	A	502	A1ETV	C13-C14-N17-C18
2	E	501	A1ETV	C13-C14-N17-C18
2	A	501	A1ETV	C13-C14-N17-C19
2	A	501	A1ETV	C15-C14-N17-C18
2	A	502	A1ETV	C13-C14-N17-C19
2	A	502	A1ETV	C15-C14-N17-C18
2	E	501	A1ETV	C13-C14-N17-C19

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Mol	Chain	Res	Type	Atoms
2	E	501	A1ETV	C15-C14-N17-C18

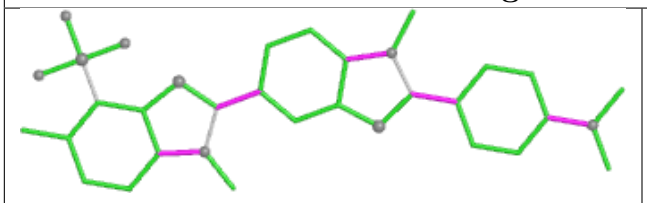
There are no ring outliers.

3 monomers are involved in 16 short contacts:

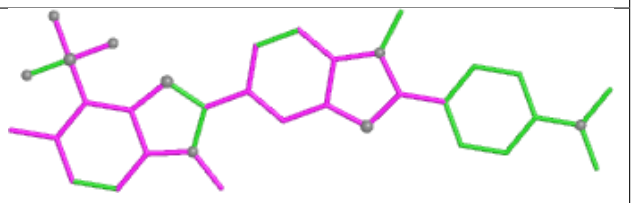
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	A1ETV	8	0
2	E	501	A1ETV	2	0
2	A	501	A1ETV	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

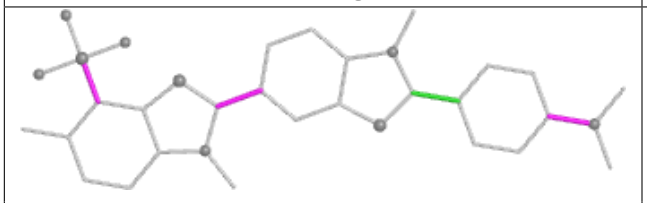
Ligand A1ETV A 502



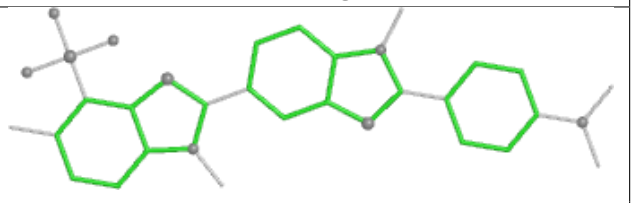
Bond lengths



Bond angles

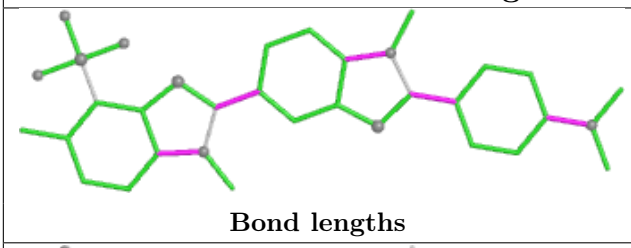


Torsions

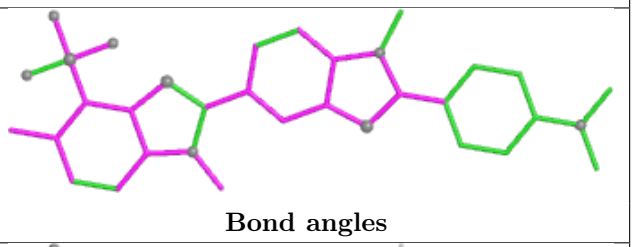


Rings

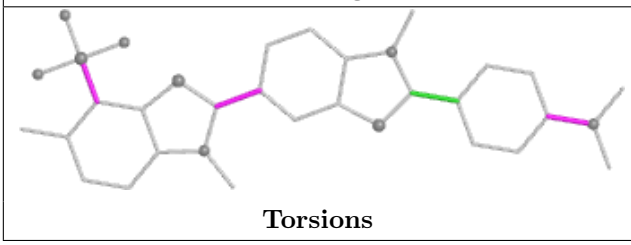
Ligand A1ETV E 501



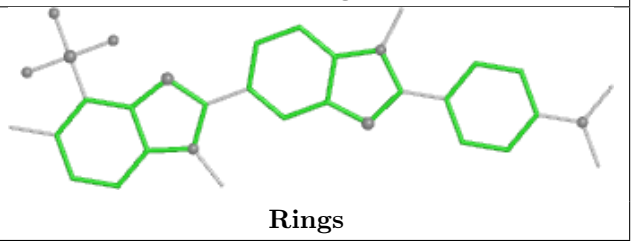
Bond lengths



Bond angles

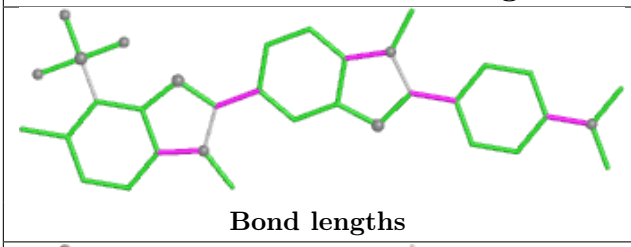


Torsions

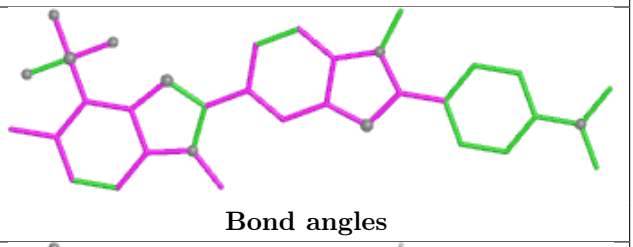


Rings

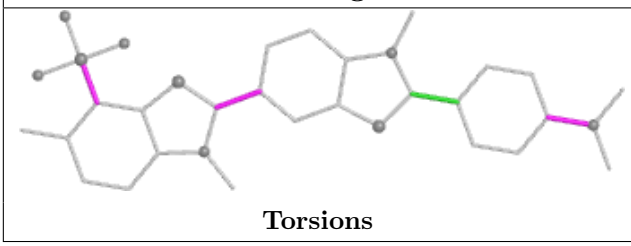
Ligand A1ETV A 501



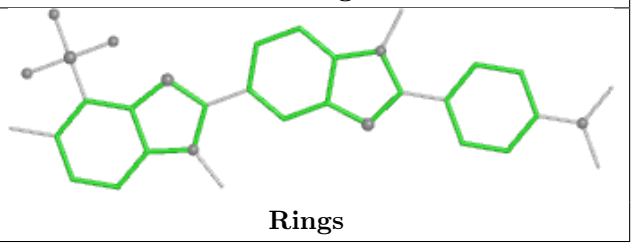
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

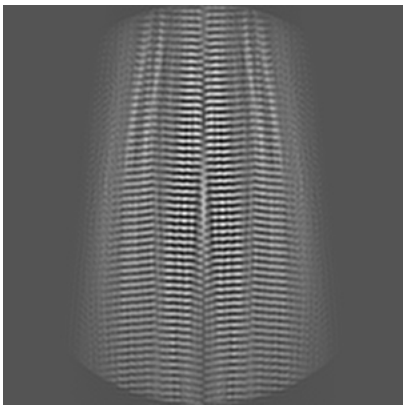
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66886. These allow visual inspection of the internal detail of the map and identification of artifacts.

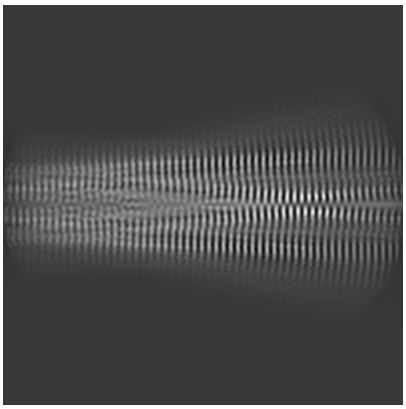
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

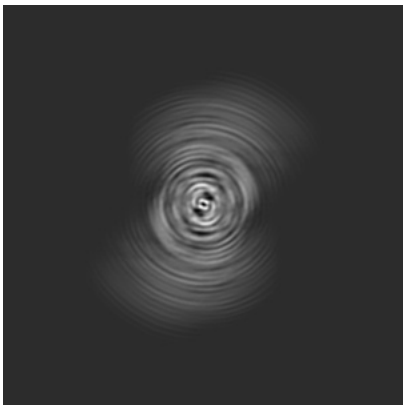
6.1.1 Primary map



X

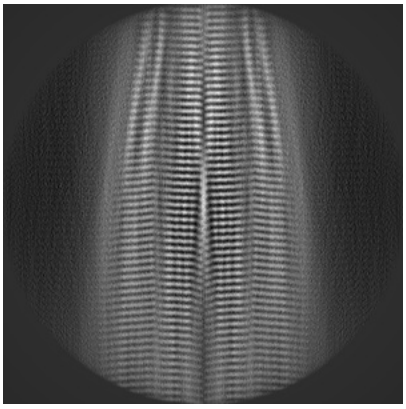


Y

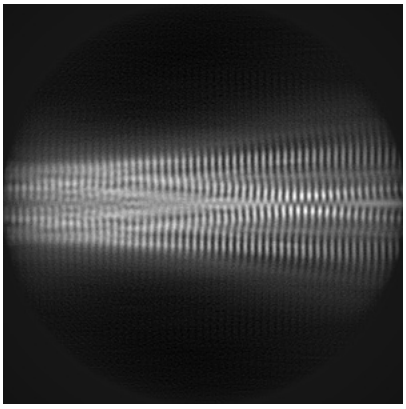


Z

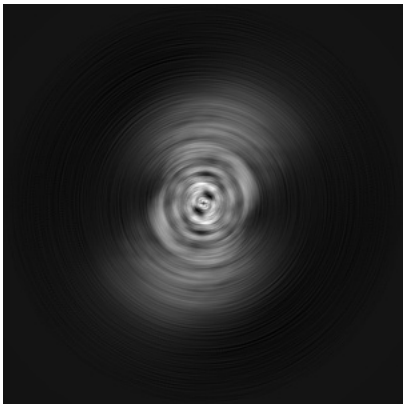
6.1.2 Raw map



X



Y

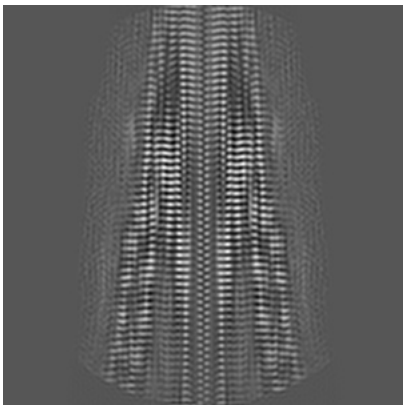


Z

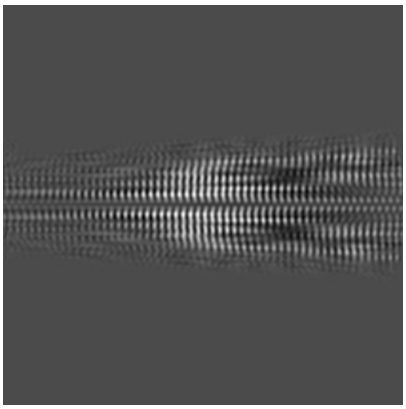
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

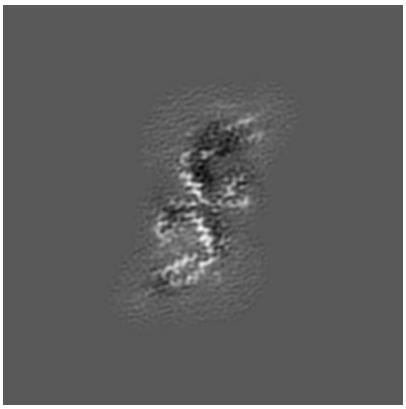
6.2.1 Primary map



X Index: 160

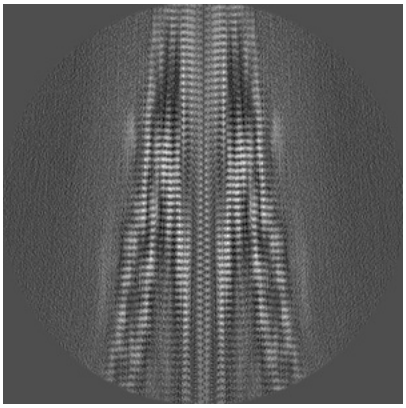


Y Index: 160

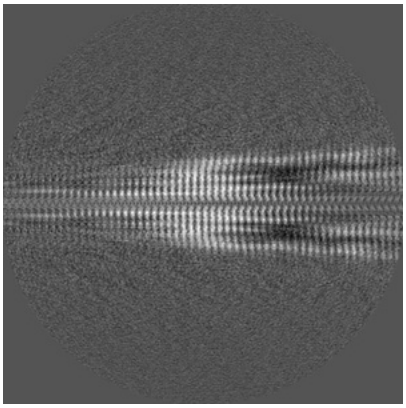


Z Index: 160

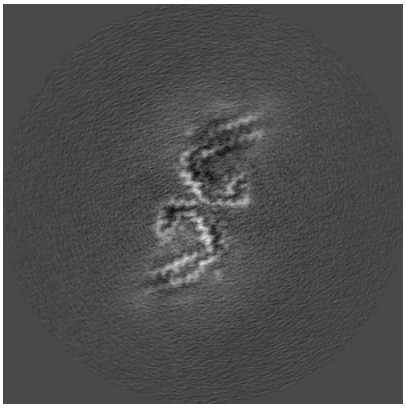
6.2.2 Raw map



X Index: 160



Y Index: 160

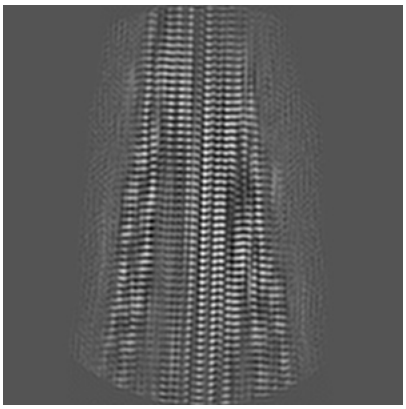


Z Index: 160

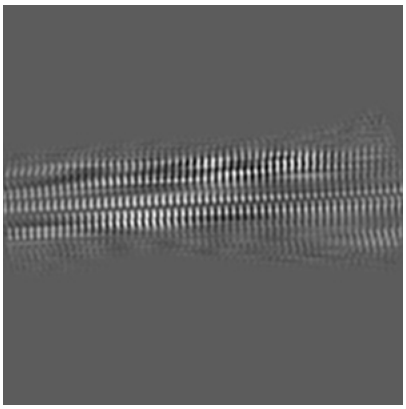
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

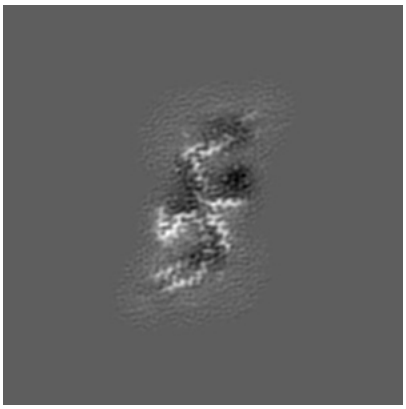
6.3.1 Primary map



X Index: 152

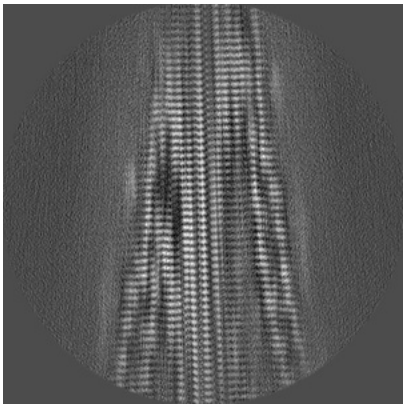


Y Index: 174

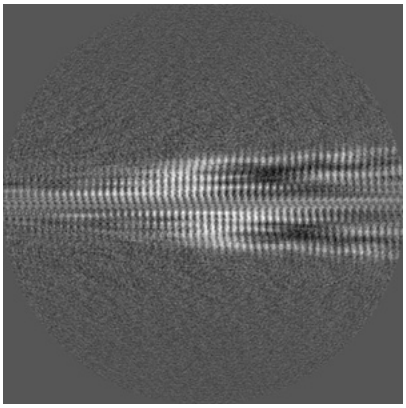


Z Index: 147

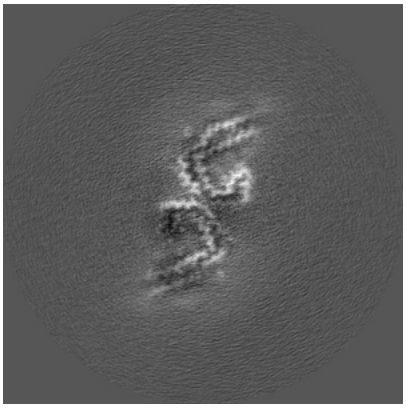
6.3.2 Raw map



X Index: 168



Y Index: 161

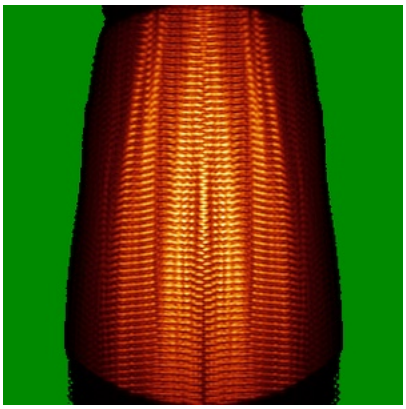


Z Index: 150

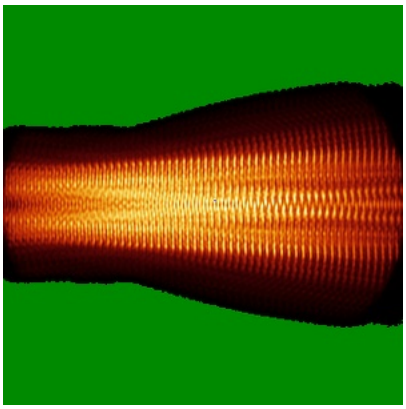
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

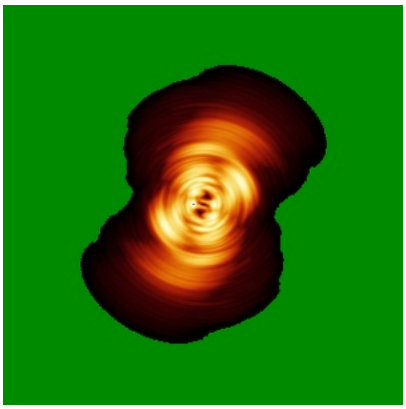
6.4.1 Primary map



X

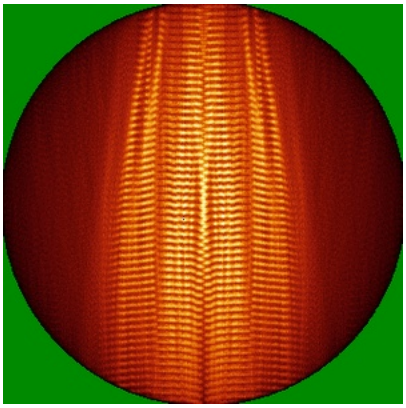


Y

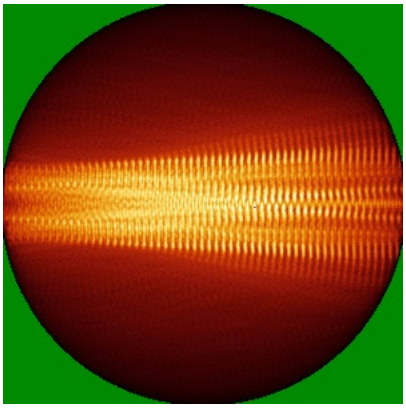


Z

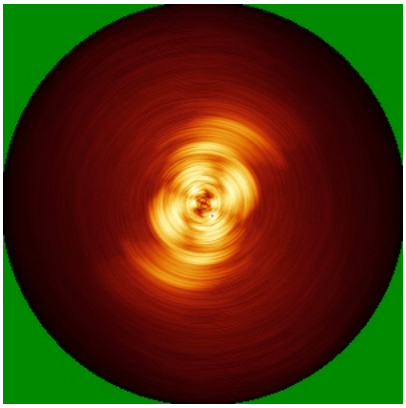
6.4.2 Raw map



X



Y

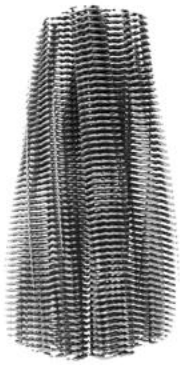


Z

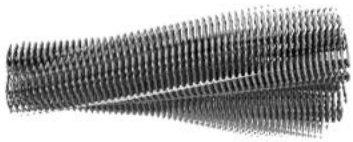
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X



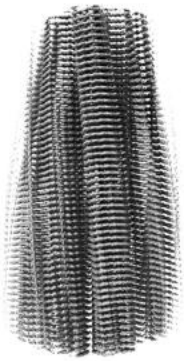
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0041. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

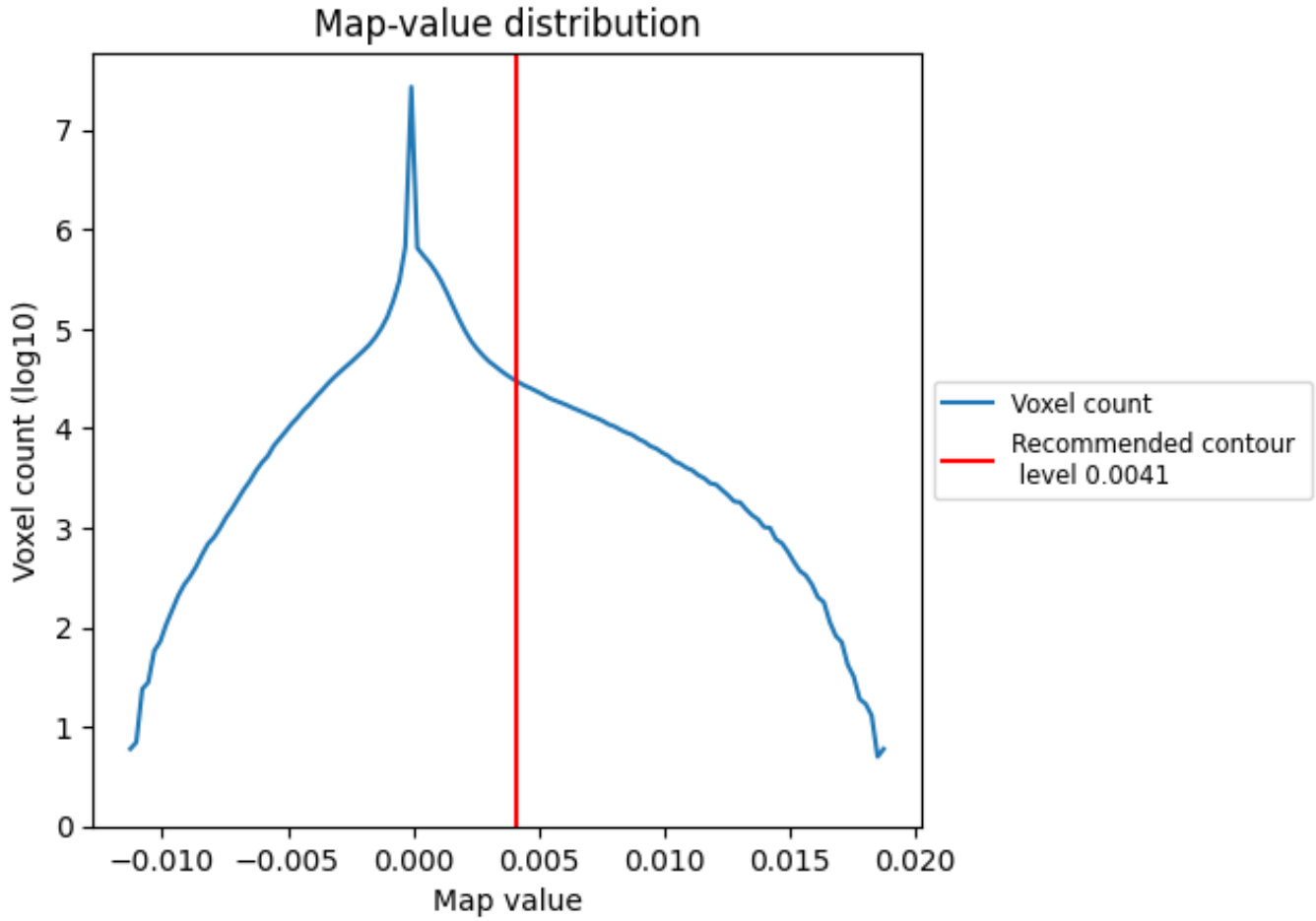
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

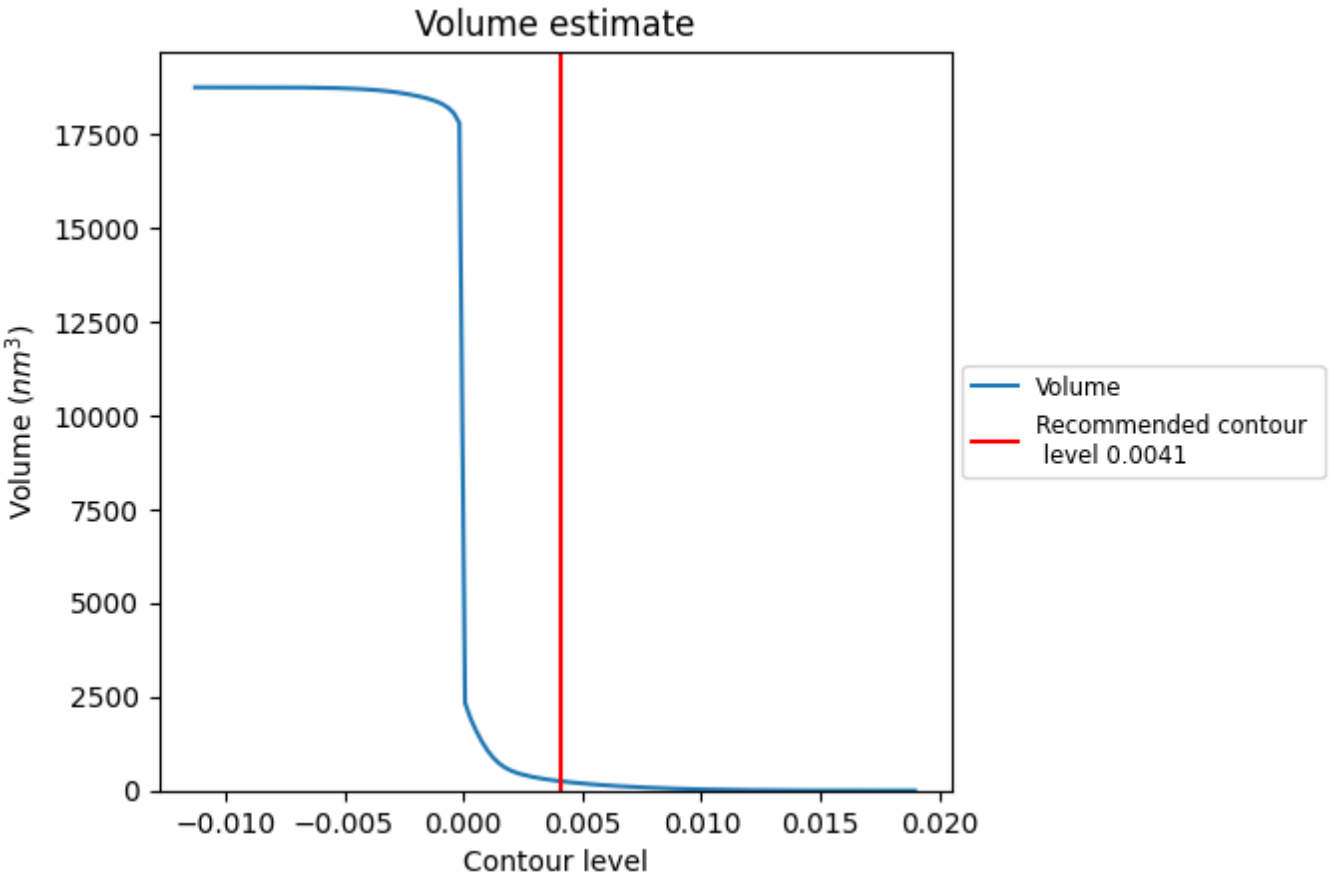
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

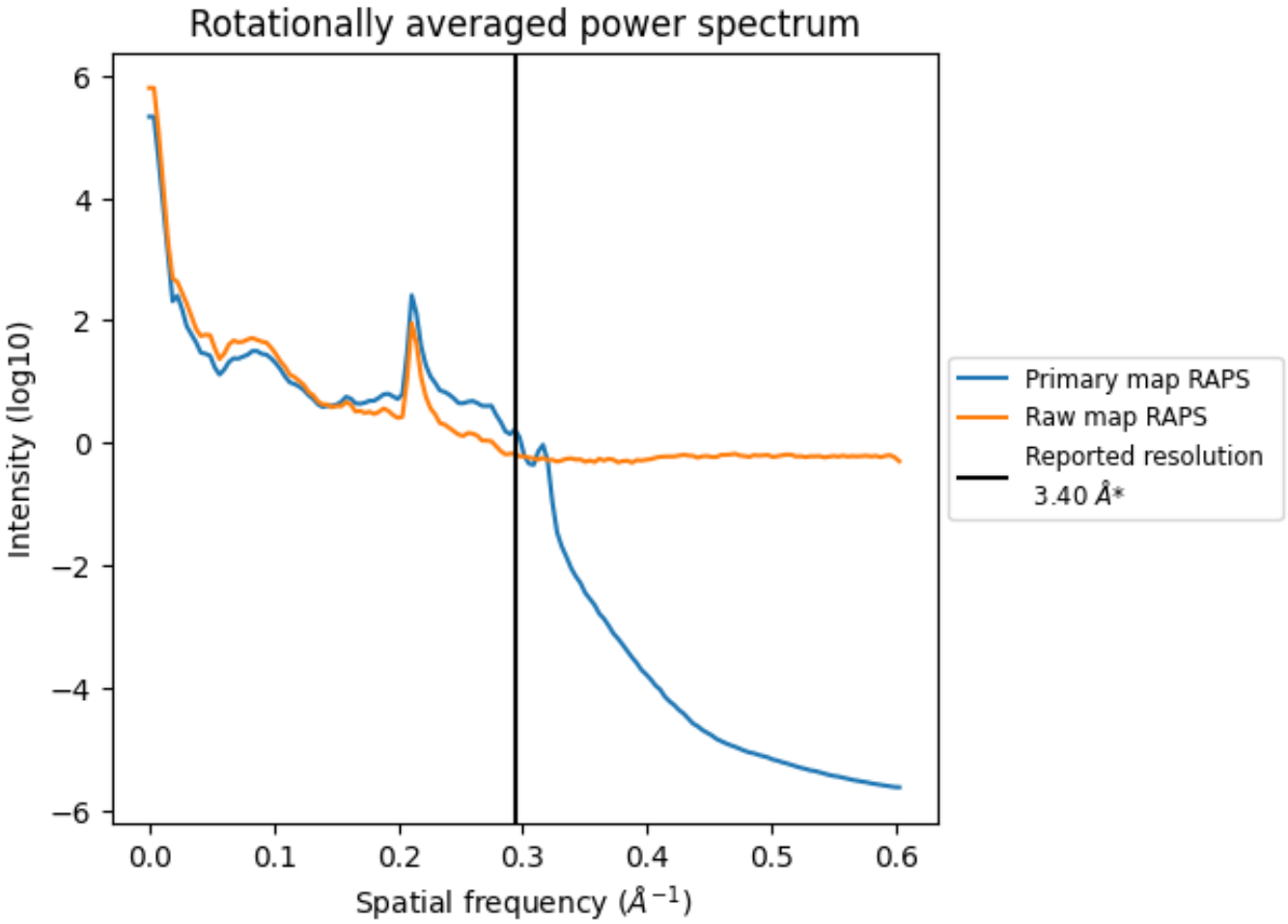
7.2 Volume estimate (i)



The volume at the recommended contour level is 248 nm^3; this corresponds to an approximate mass of 224 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

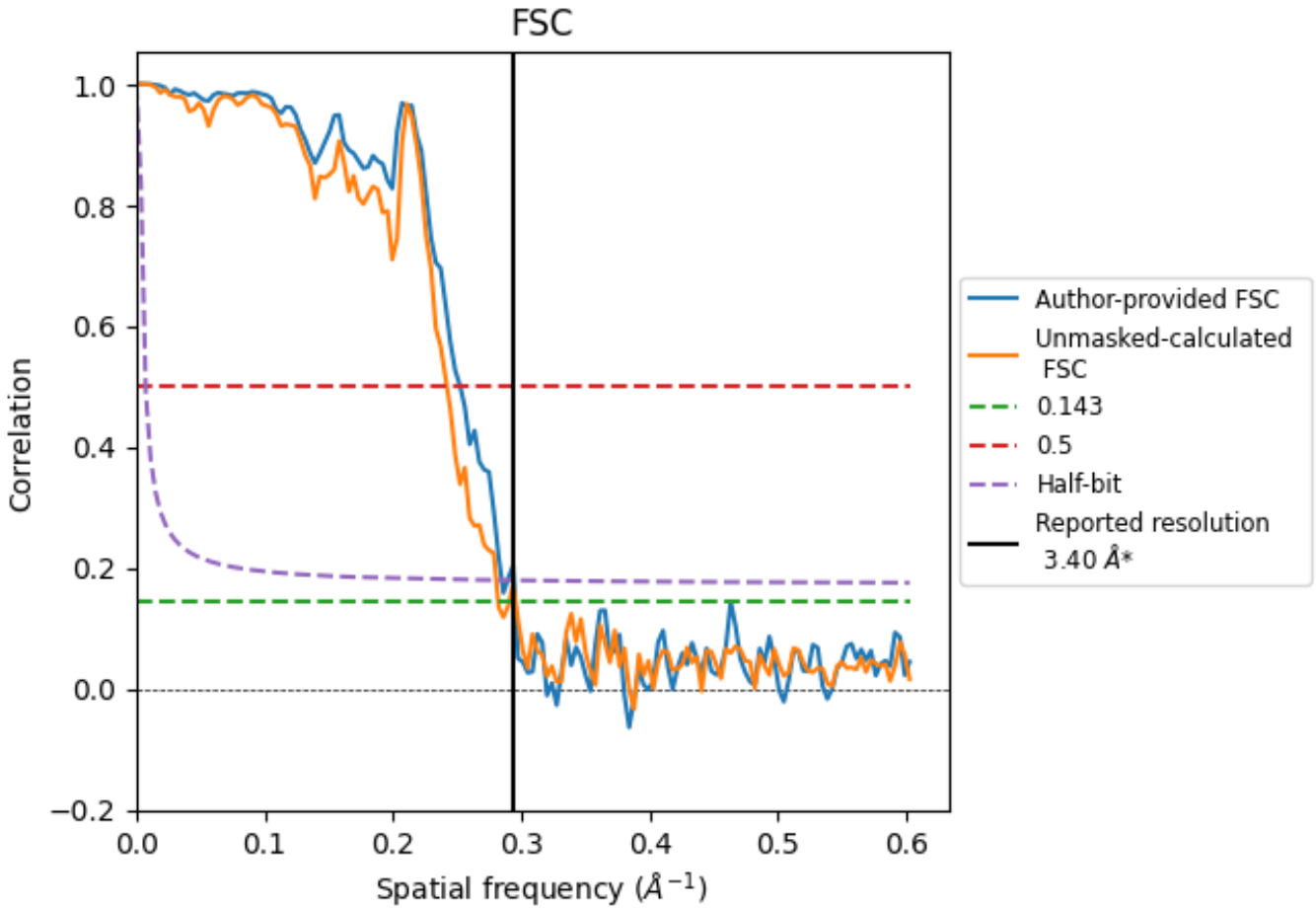


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.39	3.96	3.51
Unmasked-calculated*	3.55	4.13	3.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

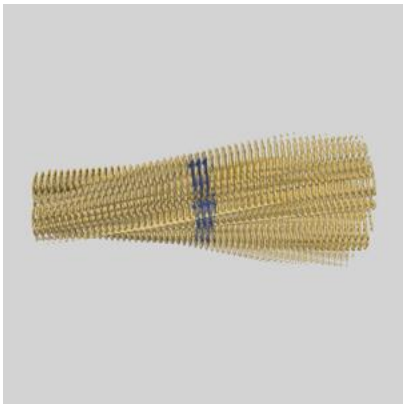
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66886 and PDB model 9XHU. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay



X



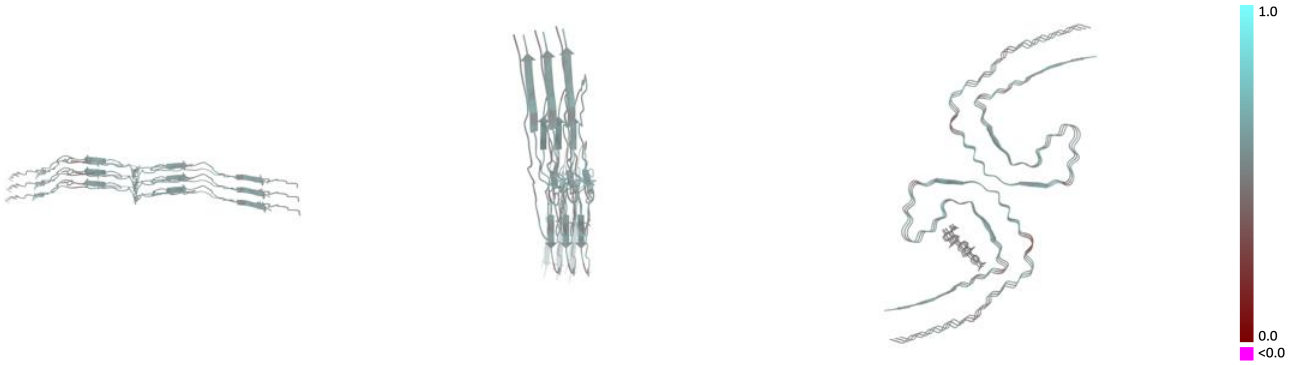
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0041 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

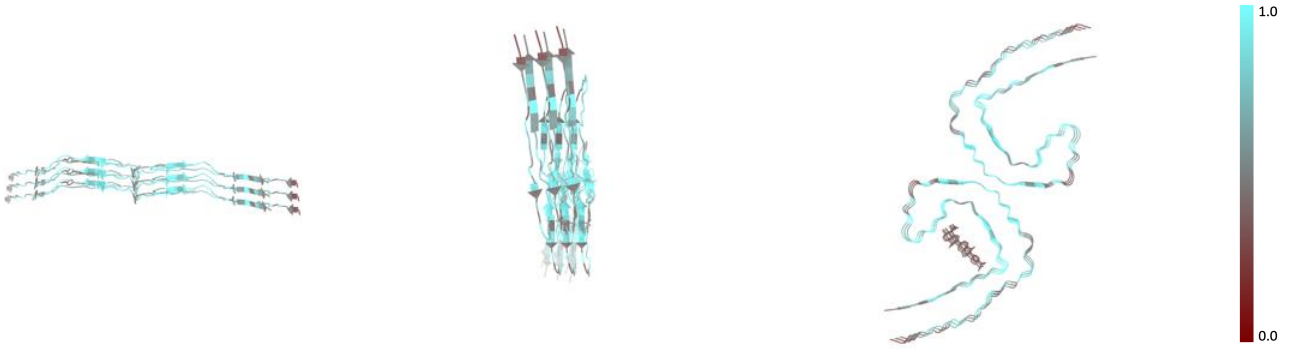
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

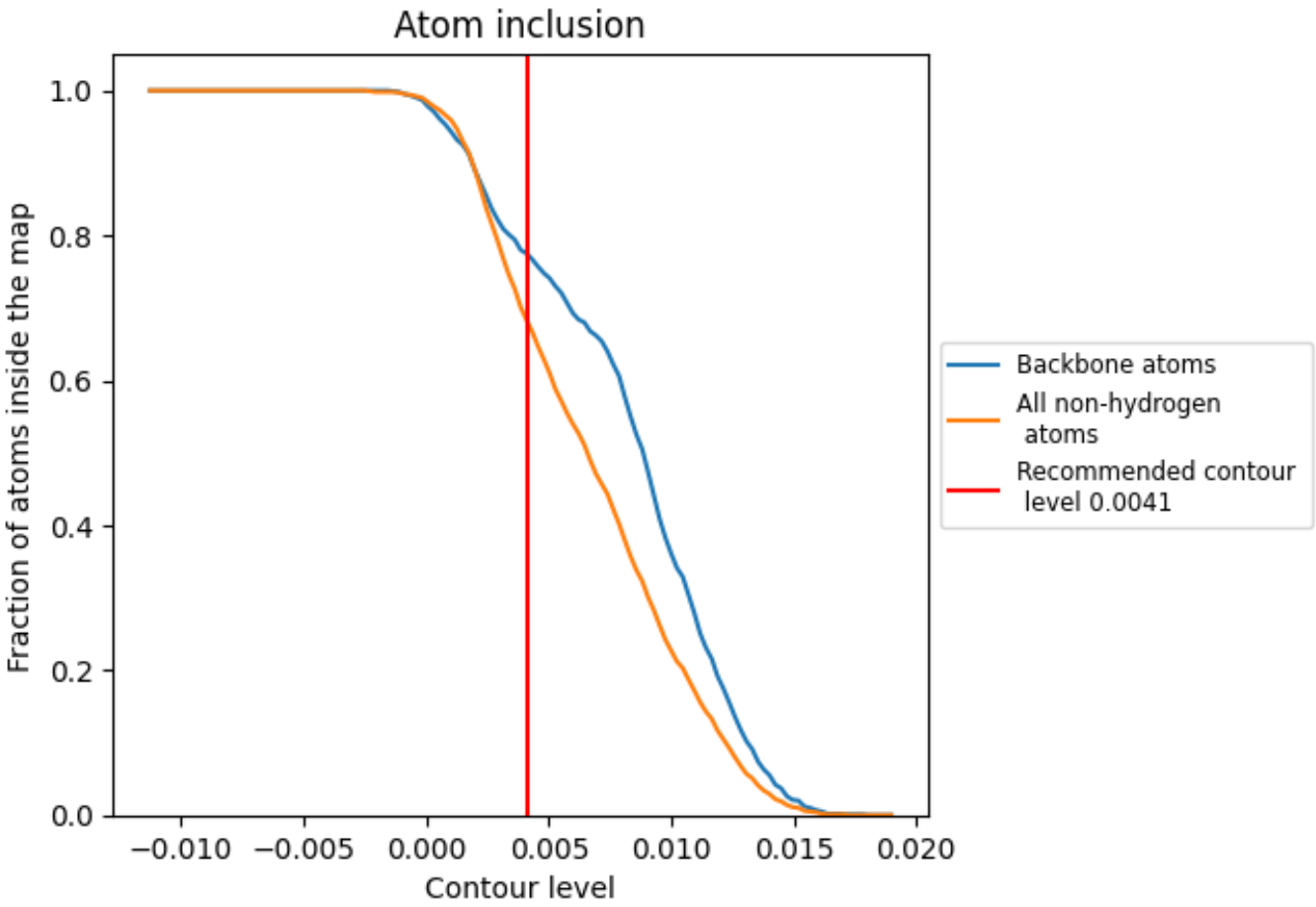
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0041).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0041) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.5270
A	0.6500	0.5210
B	0.6890	0.5310
C	0.6930	0.5260
D	0.7000	0.5310
E	0.6780	0.5230
F	0.6930	0.5300

